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Lorentz factor for triple-axis spectrometers.* By R. Pynn, *Brookhaven National Laboratory, Upton, New York* 11973, *U.S.A.*

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An expression for the Lorentz factor relevant to a triple-axis neutron spectrometer is presented. The expression relates the structure factor of a Bragg peak to the integrated intensity obtained with any scan which passes through the Bragg point and which follows a linear path in reciprocal space. The important exact result obtained here is that the Lorentz factor is the same for double-axis and triple-axis spectrometers when a θ–2θ scan is used and when the sample is a single crystal with a narrow mosaic.

In a neutron diffraction experiment the measured, integrated intensity of a Bragg reflection is related to the structure factor of the reflection by the Lorentz factor (Marshall & Lovesey, 1971; Azároff, 1968). This factor depends on both the scattering angle and the type of scan used (Yessik, Werner & Sato, 1973). For the conventional situation of a θ–2θ scan (scattering and sample angles coupled in a two-to-one ratio) with a double-axis spectrometer, one finds for a single-crystal sample that (Iizumi, 1973)

$$I \propto \frac{1}{\sin 2\theta_s} \cdot |F|^2. \quad (1)$$

Here I is the intensity integrated over the scattering angle $2\theta_s$ and F is the structure factor of the Bragg reflection in question.

The two-axis instrument alluded to above is often not the most suitable for measuring Bragg intensity. If the structure factor of a Bragg reflection is small, an improved signal-to-noise ratio may be obtained by using a triple-axis spectrometer. In addition to reducing the background, the use of an analyzer crystal and of detector collimation may help to reduce the effects of multiple scattering contamination. In order to make full use of these advantages the Lorentz factor for scans performed with a triple-axis instrument must be known; they are presented in this communication.

Consider an arbitrary linear scan in reciprocal space defined by the equation

$$\alpha Q_{ox} + \beta Q_{oy} = 0; \quad Q_{oz} = 0 \quad (2)$$

where $(Q_{ox}, Q_{oy}, Q_{oz}) \equiv \mathbf{Q}_0$ is a wave vector somewhere on the scan. In equation (2) the coordinate system is that chosen by Cooper & Nathans (1967) in which Q_{ox} coincides in direction with the negative of the neutron scattering vector (*cf.* Fig. 1). Q_{ox}, Q_{oy}, and Q_{oz} are measured from the Bragg point which is to be scanned. As particular examples drawn from equation (2) one may note that the combination $\alpha=0$, $\beta=1$ corresponds to a θ–2θ scan while $\alpha=1$, $\beta=0$ corresponds to a rotation of the sample axis only (φ scan†).

Suppose that the intensity profile of the Bragg peak scanned according to equation (2) is plotted as a function of the distance $|\mathbf{Q}_0|$ from the Bragg peak. The integrated intensity, or area under the profile, is given by

$$I \propto \int d^3Q_0 \int d^3Q R(\mathbf{Q}-\mathbf{Q}_0)\delta(\mathbf{Q})\delta(\alpha Q_{ox}+\beta Q_{oy})\delta(Q_{oz})|F|^2 \quad (3)$$

where $R(\mathbf{Q}-\mathbf{Q}_0)$ is the (zero-energy) spectrometer resolution function discussed by Cooper & Nathans (1967). If one assumes that the parameters which define $R(\mathbf{Q}-\mathbf{Q}_0)$ depend only weakly on $\mathbf{Q}_0$, and that the resolution function is therefore approximately constant during a scan, one may show that:

$$I \propto |F|^2/[k^3 \sin\theta_s \,.\, V_0 Q_B^2 \sqrt{C\alpha_s\beta_s} \times \sqrt{(\beta^2 M'_{11} + \alpha^2 M'_{22} - 2\alpha\beta M'_{12})}] \quad (4)$$

where k is the neutron wave vector $(=2\pi/\lambda)$, $C=(1/\beta_1^2+1/\beta_2^2)k^2$, β_1,β_2 are vertical collimations before and after the sample, Q_B is the reciprocal lattice vector of the Bragg reflection scanned, $Q_B^2\alpha_s = 1/\eta_{SH}^2 + Q_B^2 M_{22}$, $Q_B^2\beta_s = 1/\eta_{SV}^2 + Q_B^2 M_{33}$, η_{SH}, η_{SV} are horizontal and vertical mosaics of the sample, M_{ij} are elements of the spectrometer resolution matrix.

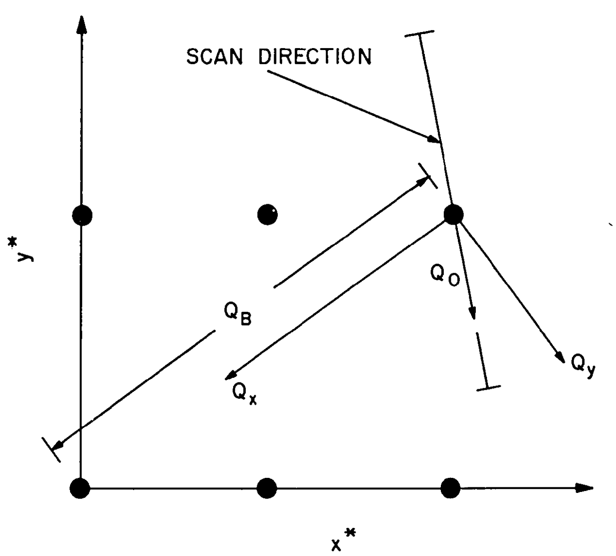

Fig. 1. Reciprocal lattice of sample with Bragg points shown as filled circles. The coordinate axis Q_z is perpendicular to the plane of the figure.

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† The term 'φ scan' is used here to denote a scan in which the sample is rotated about an axis perpendicular to the scattering plane. Alternative, frequently used designations for this type of scan are 'ω scan' and 'θ scan'.

Expressions for M'_{ij} and V_0 are given in the paper by Werner & Pynn (1971) for the case of relaxed in-pile and detector collimations. Briefly one has

$$M_{ij} = \mathbf{V}_i \,.\, \mathbf{V}_j - (\mathbf{V}_0 \,.\, \mathbf{V}_i)\,(\mathbf{V}_0 \,.\, \mathbf{V}_j)/|V_0|^2$$

$$M'_{ij} = M_{ij} - M_{i2}M_{j2}/\alpha_s \quad \text{for } i \text{ and } j = 1,2,4 \tag{5}$$

$$M'_{33} = M_{33} - M^2_{33}/\beta_s$$

and

$$\mathbf{V}_j \equiv (s_j, r_j, p_j, q_j)$$

where $s_j \ldots q_j$ are defined by Werner & Pynn (1971) in terms of the spectrometer variables (collimations, mosaics, *etc.*). To include horizontal in-pile and detector collimations one must write

$$\mathbf{V}_j \equiv (s_j, r_j, p_j, q_j, n_j, m_j) \tag{6}$$

with

$$n_0 = B/\alpha_3 k$$

$$n_1 = -Au_1/\alpha_3 k$$

$$n_2 = -Au_2/\alpha_3 k$$

$$m_0 = (b/k + 2T_m a)/\alpha_0$$

$$m_1 = (-a/k + 2T_m b)\,(u_1 - 1)/\alpha_0$$

$$m_2 = (-au_2/k - b/k + 2T_m bu_2 - 2T_m a)/\alpha_0$$

where B, A, u_1, u_2, b, a and T_m are defined by Werner & Pynn (1971) and α_0 and α_3 are horizontal in-pile and detector collimations respectively.

In general, equation (4) must be evaluated for each case of interest. However, in the limit of vanishing sample mosaic a number of useful exact results may be derived. In particular, one finds in this limit, and for a θ–2θ scan, that the integrated intensity depends on the scattering angle $2\theta_s$ only through the usual $1/\sin\theta_s$ Lorentz factor which is applicable to two-axis instruments (note that $1/\sin\theta_s$ rather than $1/\sin 2\theta_s$ is the relevant factor here because integration has been performed over wave vector rather than over scattering angle). This result has recently been confirmed experimentally by Iizumi & Shirane (1975) at this laboratory.

Results computed from equation (4) for θ–2θ and φ (sample rocking curve) scans are shown in Figs. 2 and 3 for a fairly commonplace set of spectrometer parameters. The neutron energy was taken to be 14 meV, horizontal collimations (in-pile, monochromator-sample, sample-analyzer and detector) were 20′ (FWHM), vertical collimations before and after the sample were 120′ and the analyzer and monochromator crystals had mosaics of 20′ and plane spacings equal to those for the 002 reflection of pyrolytic graphite. The ordinate of both figures is the quotient of the integrated intensities obtained with double-axis, open-detector (I_2) and triple-axis (I_3) systems. Thus the horizontal line shown for $\eta_s = 0$ in Fig. 2 confirms that the same Lorentz factor applies to θ–2θ scans performed with good single crystals on both double-axis and triple-axis instruments. Notice that Fig. 3 shows that no such simple result is applicable to φ scans. In both cases, however, a good approximation to the limiting situation of $\eta_s \to 0$ appears to be rather easy to achieve experimentally.

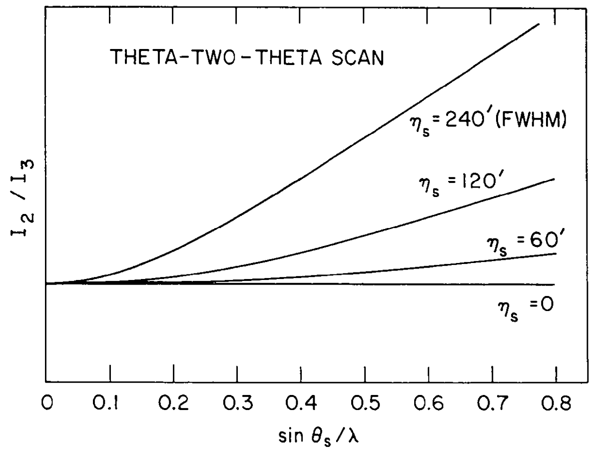

Fig. 2. The integrated intensity of an open-detector double-axis scan (I_2) divided by the integrated intensity of a triple-axis scan (I_3) plotted against sin θ_s/λ for a θ–2θ scan. Curves are drawn for various values of sample mosaic $\eta_s(=\eta_{SV}=\eta_{SH})$.

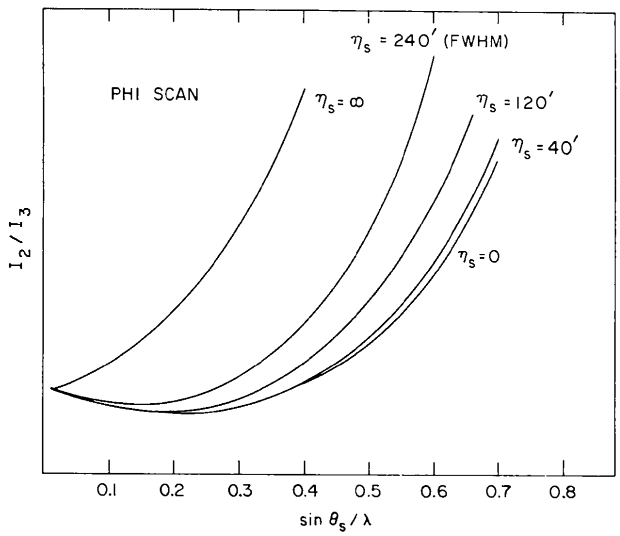

Fig. 3. The ratio I_2/I_3 (*cf.* Fig. 2) plotted against sin θ_s/λ for a φ scan (sample rocking curve). Curves are drawn for various values of sample mosaic $\eta_s(\eta_{SV}=\eta_{SH})$.

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