SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

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Lorentz factors for large-mosaic crystals. By J. D. Axe and J. B. Hastings, *Brookhaven National Laboratory, Upton, NY* 11973, *USA*

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Abstract

General expressions are derived for the Lorentz factor for two- and three-axis spectrometers to be used when the vertical resolution is comparable to or less than the mosaic of the measured Bragg reflections.

Intensities from different Bragg reflections integrated along a path s in a direction $\Delta\mathbf{Q}$ in reciprocal space are related by a Lorentz factor

$$I_{\Delta \mathbf{Q}}(\mathbf{Q}_0) \equiv \int I_{\rm Bragg}(\mathbf{Q}_0 + s\Delta\mathbf{Q})\,{\rm d}s \sim L(|Q_0|)|F(\mathbf{Q}_0)|^2. \quad (1)$$

The Lorentz factor, $L(|Q_0|) = L(\theta_s)$, depends upon the direction of the scan. For example, if the sample–detector collimation is relaxed so that the detector receives all the scattered radiation,

$$L = (\sin\theta_s)^{-1}$$

for scans parallel to $\mathbf{Q}_0$(θ–2θ scans but with equal Q steps), and

$$L = (\cos\theta_s)^{-1}$$

in scans perpendicular to $\mathbf{Q}_0$ (φ scans with equal Q steps).

Iizumi (1973) discussed the effect of horizontal collimation after the sample in a two-axis spectrometer and showed that for a θ–2θ scan, *and only for that scan*, does the Lorentz factor retain its simple form. Pynn (1975) showed numerically that even for a θ–2θ scan the simple Lorentz factor is modified with tight vertical collimation for a three-axis spectrometer. This note generalizes the above, giving explicit expressions for the modified Lorentz factors for two- or three-axis spectrometers and samples with arbitrary horizontal and vertical mosaic. The derivation, which was obtained using the formulation of Yessick, Werner & Sato (1973), is omitted.

The Lorentz factor for a θ–2θ scan (but with equal Q steps) for a mosaic sample is

$$L = \frac{f_v f_h}{\sin\theta_s}, \quad (2)$$

where

$$f_h = \left\{1 + \frac{4\eta_h^2}{\alpha_M^2 + \alpha_A^2}\right\}^{-1/2} \quad (3a)$$

$$f_v = \left\{1 + \frac{4\eta_v^2 \sin^2\theta_s}{\beta_M^2 + \beta_A^2}\right\}^{-1/2}. \quad (3b)$$

and $\eta_h(\eta_v)$ = horizontal (vertical) sample mosaic, $\alpha_M(\beta_M)$ = effective horizontal (vertical) collimation before the sample, $\alpha_A(\beta A)$ = effective horizontal (vertical) collimation after the sample.

Explicitly, for a single-crystal monochromator,

$$\alpha_M^2 = \left[\frac{1}{\alpha_0^2 + 4\eta_M^2} + \frac{1}{\alpha_1^2}\right]^{-1} \quad (4a)$$

$$\beta_M^2 = \left[\frac{1}{\beta_0^2 + 4\eta_M^2\sin^2\theta_M} + \frac{1}{\beta_1^2}\right]^{-1} \quad (4b)$$

and, for a triple-axis-analyzer section,

$$\alpha_A^2 = \left[\frac{1}{\alpha_3^2 + 4\eta_A^2} + \frac{1}{\alpha_2^2}\right]^{-1} \quad (5a)$$

$$\beta_A^2 = \left[\frac{1}{\beta_3^2 + 4\eta_A^2\sin^2\theta_A} + \frac{1}{\beta_2^2}\right]^{-1} \quad (5b)$$

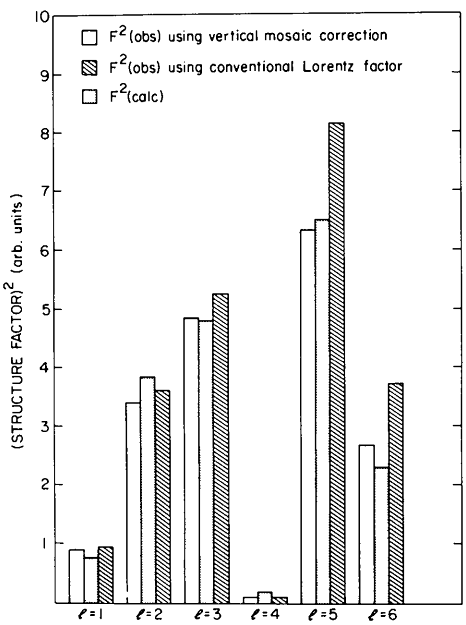

Fig. 1. Effect of vertical Lorentz correction for neutron scattering data on intercalated graphite, KC_{24}, with broad-mosaic structure.

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Collimators are specified by the subscript 0 (source–monochromator), 1 (monochromator–sample), 2 (sample–analyzer) and 3 (analyzer–detector). For a double-axis spectrometer $\alpha_3 = \beta_3 \to \infty$ in the above expressions giving

$$\alpha_A = \alpha_2 \quad \beta_A = \beta_2. \tag{5c}$$

The following points should be noted.

(*a*) f_h is independent of θ_s and can be absorbed into other constants. However, it gives a simple expression for the loss of intensity due to horizontal collimation.

(*b*) If $4\eta_v^2 > (\beta_M^2 + \beta_A^2)$ there will necessarily be a cross over from a small-Q region where

$$f_v \simeq 1, \quad L \sim \frac{1}{\sin\theta_s}$$

to a large-Q region where

$$f_v = \frac{[\beta_M^2 + \beta_A^2]^{1/2}}{2\eta_v \sin\theta_s}, \quad L \sim \frac{[\beta_M^2 + \beta_A^2]^{1/2}}{2\eta_v (\sin\theta_s)^2}.$$

In the large-Q region the θ_s dependence is identical to that for a powder sample. (One may think of f_v as the fraction of total out-of-plane scattering reaching the detector.)

(*c*) In comparing θ–2θ scans done with *equal θ step*, (2) is simply modified by replacing the factor $(\sin\theta_s)^{-1}$ by $(\sin 2\theta_s)^{-1}$.

Fig. 1 illustrates the effect of vertical Lorentz corrections for neutron scattering data taken on a stage-2 intercalated graphite compound KC_{24}. The data were taken with $\lambda = 2{\cdot}5$ Å neutrons using a triple axis spectrometer with $\beta_M \simeq 0{\cdot}7°$ and $\beta_A \simeq 1{\cdot}9°$ and the (00*l*) reflections had a measured mosaic $\eta_h = \eta_v \sim 2°$ FWHM. Note that the agreement for the high-angle reflections ($l = 5$ and 6) is considerably improved by application of the correct Lorentz factor.

References

IIZUMI, M. (1973). *Jpn. J. Appl. Phys.* **12**, 167–169.

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Acta Cryst. (1983). A**39**, 594

Statistical geometry. I. A self-consistent approach to the crystallographic inversion problem based on information theory: Erratum.

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Abstract

As a result of a printer's error, the first line of § 4.6 (page 56) of Wilkins, Varghese & Lehmann [*Acta Cryst.* (1983), A**39**, 47–60] is in error. The first sentence of that section should read: 'In order to give an illustration of the way in which the SGM may be used, ...'.

All information is given in the *Abstract*.

Acta Cryst. (1983). A**39**, 594–595

Tensor properties and rotational symmetry of crystals. III. Use of symmetrized components in group $3(3_z)$. Erratum.

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Abstract

In Fumi & Ripamonti [*Acta Cryst.* (1983), A**39**, 245–251], there are errors on page 249 in equation II(*b*) for the even-parity c^+ subtensor and II(*a*) and (*b*) for the even-parity c^- subtensor.

The correct equations are given.

Several misprints are present on page 249 of Fumi & Ripamonti (1983):

First column, equations II(*b*)

The first and third equations should read:

$$yyyyyyxx^+ = c_1\,\overset{15}{\overline{yyyyxxxx}}{}^+ + c_2\,\overset{20}{\overline{yyyxxxyx}}{}^+$$

$$yyyyyyxx^+ = \tfrac{1}{3}\,\overset{15}{\overline{yyyyxxxx}}{}^+ - \tfrac{1}{6}\,\overset{20}{\overline{yyyxxxyx}}{}^+.$$

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