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The inversion of three-beam intensities for scalar scattering by a general centrosymmetric crystal. By

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Abstract

It is shown that, for the general centrosymmetric crystal, both the signs and magnitudes of all structure amplitudes may be obtained uniquely and explicitly from an analysis of the variation with angle of incidence of the three-beam elastic intensities. The solution derives from certain symmetries which are shown to be inherent in the three-beam dynamical wavefunction.

Within the approximations of one-beam (kinematical) and two-beam diffraction, structure amplitudes, but not phases, can be determined directly; while in the three-beam approximation, and for centrosymmetric crystals, phases, but not all amplitudes, have been determined (Kambe, 1957*a*,*b*; Hart & Lang, 1961; Goodman, 1973; Post, 1979). It is the purpose of this note to show that, for centrosymmetic crystals, and within the approximation of three-beam elastic scattering, a prescription can be provided for the determination of all amplitudes and phases uniquely and directly from the distribution of scattered intensity.

The method depends on finding all orientations for which the intensity of a specific beam, say beam h, can take two-beam form, that is, in finding all angles of incidence for which $I_h = V_h^2(\sin^2 bz)/b^2$, where z is the thickness of the crystal, b is to be determined, and V_h is a scattering amplitude in which, for brevity, the appropriate constant (conventionally σ) has been absorbed. It is emphasized that this condition is imposed on only one beam at a time, a requirement less restrictive than that for confluence.

Writing the scattering matrix in terms of projection operators (Hurley, Johnson, Moodie, Rez & Sellar, 1978), and making standard substitutions of the type $\lambda = \omega v + \omega^2 v^*$ for the roots of the reduced characteristic equation, we get, after some algebra, the wavefunction

$$\begin{aligned} &u_h \exp[-\tfrac{1}{3}i(\zeta_h + \zeta_g)z] \exp[i(\alpha/3)z] \\ &= iV_h \sin\beta z/\beta - [\tfrac{1}{3}(\zeta_h - 2\zeta_g + 2\alpha)V_h + V_g V_{g-h}] \\ &\quad \times \frac{[\beta(\cos\beta z - \cos\alpha z) + i(\alpha\sin\beta z - \beta\sin\alpha z)]}{\beta(\alpha^2 - \beta^2)}, \end{aligned}$$

where $v + v^* = \frac{2}{3}\alpha$, $v - v^* = i2\beta/\sqrt{3}$; u_h is the wavefunction of the beam h, and ζ_h, ζ_g are excitation errors with the factor 2π absorbed for compactness.

Thus, in general centrosymmetric crystals, the beam h is of two-beam form if and only if

$$\lambda = \tfrac{1}{3}(2\zeta_g - \zeta_h) - V_g V_{g-h}/V_h. \qquad (1)$$

Since λ must satisfy the characteristic equation, the condition of (1), at arbitrary wavelength, imposes a relationship on ζ_h, ζ_g. Specifically, ζ_h, ζ_g are constrained to lie on the degenerate hyperbola

$$\left[\zeta_g - \frac{V_g}{V_h V_{g-h}}(V_{g-h}^2 - V_h^2)\right] \times \left[\zeta_g - \zeta_h - \frac{V_{g-h}}{V_h V_g}(V_g^2 - V_h^2)\right] = 0,$$

that is either on a line (a) or on a line (b).

These lines intersect at the 'Gjønnes point' (Gjønnes & Høier, 1971) of confluence with ζ_h, ζ_g given by

$$G_1 = \frac{V_h}{V_g V_{g-h}}(V_{g-h}^2 - V_g^2),$$

$$G_2 = \frac{V_g}{V_h V_{g-h}}(V_{g-h}^2 - V_h^2).$$

Along the line (a),

$$\zeta_g = \frac{V_g}{V_h V_{g-h}}(V_{g-h}^2 - V_h^2),$$

$$I_h = V_h^2 \frac{\sin^2\beta_1 z}{\beta_1^2},$$

where

$$\beta_1 = \tfrac{1}{2}\left[\left(\zeta_h - \frac{V_g V_{g-h}}{V_h}\right)^2 + 4(V_{g-h}^2 + V_h^2)\right]^{1/2},$$

while along the line (b),

$$\zeta_g = \zeta_h + \frac{V_{g-h}}{V_h V_g}(V_g^2 - V_h^2),$$

$$I_h = V_h^2 \frac{\sin^2\beta_2 z}{\beta_2^2},$$

where

$$\beta_2 = \frac{1}{2}\left[\left(\zeta_h + \frac{V_g V_{g-h}}{V_h}\right)^2 + 4(V_g^2 + V_h^2)\right]^{1/2}$$

The centres of the two-beam distributions are therefore displaced equal and opposite distances, $G_3 = V_g V_{g-h}/V_h$, along the ζ_h axis.

The pair of lines in beam g is obtained by interchanging the subscripts h and g, an interchange which leaves line (b) invariant (Fig. 1). In the central beam there is only one symmetry line, namely (b).

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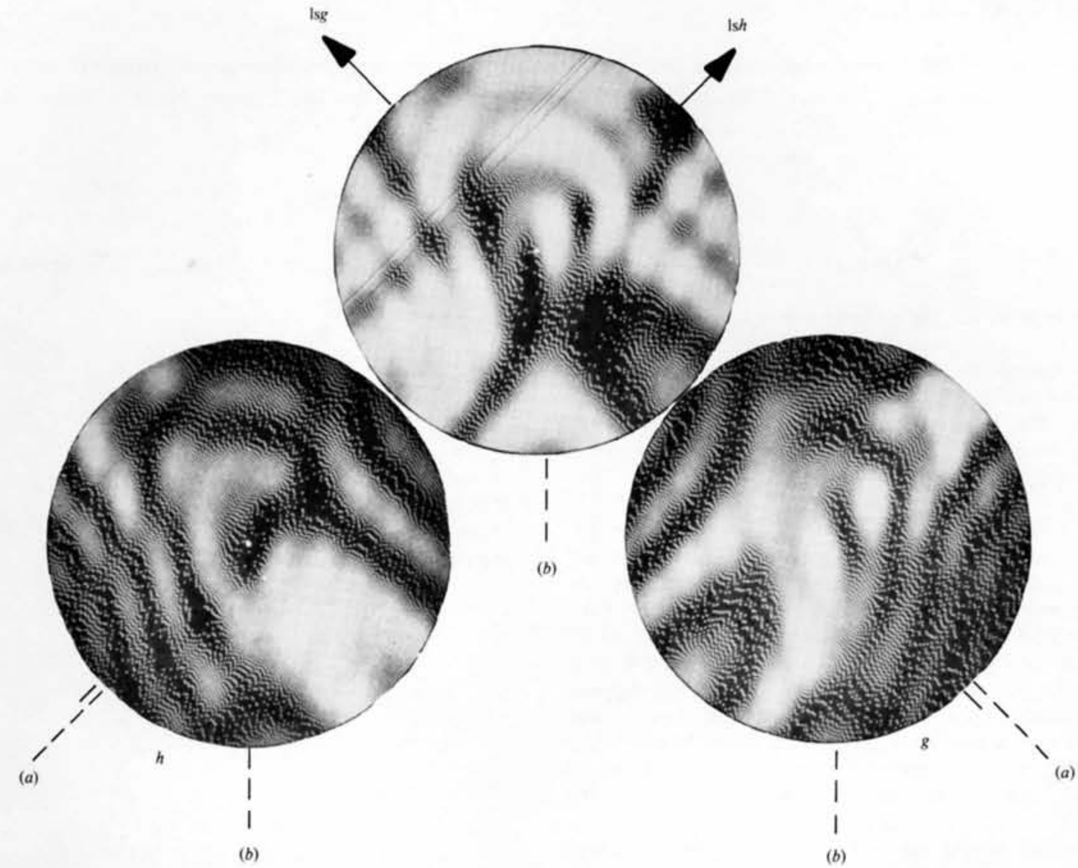

Fig. 1 Analogue computation (Johnson, 1968) of a three-beam diffraction pattern indicating the lines of two-beam form which lead to inversion; $V_h = 0{\cdot}9, V_g = 0{\cdot}7$ and $V_{g-h} = 0{\cdot}8$. The central markers in each disc correspond to the exact Bragg condition.

Thus, in a three-beam convergent-beam diffraction pattern, the unique symmetry lines are identified in the disc of either diffracted beam, and hence G_1, G_2 and G_3 are obtained; the sign of G_3 phases the structure amplitudes, and

$$V_h^2 = (G_3 - G_2)(G_3 - G_2 + G_1),$$

$$V_g^2 = G_3(G_3 - G_2),$$

$$V_{g-h}^2 = G_3(G_3 - G_2 + G_1),$$

which completes the inversion. The other diffracted beam, and the central beam provide checks. The result is independent of thickness.

'Critical voltage' expressions can be obtained as special cases of the above equations. This, and other extensions, will be discussed in a further publication.

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