the definition (43) leaves $S^{(r)}(\mathbf{x})$ m-dimensional, but it is clear that the subsequent transformation of $S^{(r)}(\mathbf{x})$ under $\mathbf{A}_2$ requires the transformation of an $(m-r)$-dimensional δ-function as in § 2. The equivalence of $(\mathbf{A}_1\mathbf{A}_2)S$ and $\mathbf{A}_1(\mathbf{A}_2S)$ with $\mathbf{A}_1$ singular should follow for the same reason.

(iii) In so far as the point sets of (8) are idealizations of a real situation in which electron density $S(\mathbf{x})>0$ at almost all points of space, it is natural to enquire how far the operations of convolution and affine transformation commute for general sets $S(\mathbf{x})$. If $\mathbf{T}$ is non-singular and $S^*=\mathbf{T}S$ is defined as in (6), it is clear from the argument leading to (7) that more generally

$$\mathbf{T}(\widehat{S_1S_2}) \equiv \widehat{S_1^*S_2^*} \qquad (44)$$

for all integrable sets S_1, S_2 for which the convolution $\widehat{S_1S_2}$ exists. The following is a proof of (44) when $\mathbf{T}$ is singular and S_1 and S_2 are not periodic and have convergent integrals, that is have finite total weights.

By a proper choice of basis in the m-dimensional space, $\mathbf{A}$ of rank $r<m$ is completely reduced to $\mathbf{A}^{(r)}+\mathbf{A}^{(m-r)}$, where $\mathbf{A}^{(m-r)}=\mathbf{0}^{(m-r)}$. Let now

$$g(\mathbf{x}^{(r)}) = \int S(\mathbf{x})\,d\mathbf{x}^{(m-r)}.$$

Then using (43) and the interpretation (6)

$$S_1^*=|\det \mathbf{A}^{(r)}|^{-1}g_1((\mathbf{A}^{(r)})^{-1}\mathbf{x}^{(r)})\delta(\mathbf{x}^{(m-r)})\ ,$$

since from (8) to (9)

$$\mathbf{0}^{(m-r)}\delta(\mathbf{x}^{(m-r)})=\delta(\mathbf{x}^{(m-r)})\ .$$

Then

$$\widehat{S_1^*S_2^*} = \{\mathbf{A}^{(r)}\widehat{g_1g_2}\}\delta(\mathbf{x}^{(m-r)})\ .$$

Also

$$\begin{aligned}\mathbf{A}\widehat{S_1S_2} &= \left\{\mathbf{A}^{(r)}\iint S_1(\mathbf{y})S_2(\mathbf{x}-\mathbf{y})\,d\mathbf{y}\,d\mathbf{x}^{(m-r)}\right\}\delta(\mathbf{x}^{(m-r)})\\ &= \left\{\mathbf{A}^{(r)}\int S_1(\mathbf{y})\int S_2(\mathbf{x}-\mathbf{y})\,d(\mathbf{x}-\mathbf{y})^{(m-r)}\,d\mathbf{y}\right\}\delta(\mathbf{x}^{(m-r)})\\ &= \{\mathbf{A}^{(r)}\widehat{g_1g_2}\}\delta(\mathbf{x}^{(m-r)})\end{aligned}$$

which proves the theorem.

The reversal of the integrations puts certain further conditions on S_1 and S_2; *e.g.* sufficient conditions would be continuity of these functions and uniform convergence of their integrals if the range of integration is all space or all of some infinite sub-space. These conditions obtain for any real distribution of electron density.

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Short Communications

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General spot-size correction for inclined incident beam: Weissenberg method.

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D. C. Phillips (1954, 1956) has derived formulae giving the reflexion spot area variations observed on upper-level Weissenberg photographs. These apply only to the normal-beam and equi-inclination methods. Since the formulae involve the axial coordinate ζ which is dependent upon the wave-length, it follows that the Phillips correction cannot be applied to $K\beta$ spots if the incident beam is set in the equi-inclination position for the $K\alpha$ radiation. It is sometimes, however, very desirable to make use of the intensities of the $K\beta$ spots, for example if the $K\alpha$ are too strong, if they are just outside the limiting sphere or if they are enhanced by the Renninger effect. It seems necessary, therefore, to give the Phillips equations for the general case.

The nomenclature used is that of section 4·3 of the *International Tables for X-ray Crystallography* (hereinafter *I.T.*) Volume II (1959), which differs from that of Phillips mainly in using φ for the angular coordinate instead of ω. The method consists in determining the reflexion-spot length $\mathfrak{L}$ (parallel to the rotation axis) without any camera translation; and then of determining the additional $\pm\Delta\mathfrak{L}$ introduced by the movement of the camera during the crystal rotation $\Delta\varphi$. The angular divergence of the primary beam is taken as 2α, μ is the inclination of the primary beam to the equatorial plane, ν is the angle between the nth layer-line generator and the equatorial plane.

Determination of reflexion-spot length $\mathfrak{L}$ on a stationary cylindrical film, radius r_1, axis parallel to rotation axis

The mean and limiting reflexion cones have semi-vertical angles $\frac{1}{2}\pi-\nu$, $\frac{1}{2}\pi-\nu_1$, $\frac{1}{2}\pi-\nu_2$ where $\sin\nu=\zeta+\sin\mu$ (equation (1), p. 175, *I.T.* Vol. II)

$$\sin\nu_1=\zeta+\sin(\mu+\alpha)=\sin\nu+\alpha\cos\mu$$

since α is small

$$\sin\nu_2=\zeta+\sin(\mu-\alpha)=\sin\nu-\alpha\cos\mu\ .$$

Then

$$\mathfrak{L}=r_1(\tan\nu_1-\tan\nu_2)+l$$

where

$$l=2\alpha r_0\sec\mu$$

is the length of the crystal element† (r_0 = divergent-beam 'source' to crystal distance).

$$\mathfrak{L}=r_1\left[\frac{\sin\nu_1}{(1-\sin^2\nu_1)^{\frac{1}{2}}}-\frac{\sin\nu_2}{(1-\sin^2\nu_2)^{\frac{1}{2}}}\right]+l$$

$$=r_1\left[\frac{(\sin^2\nu_1-\sin^2\nu_1\sin^2\nu_2)^{\frac{1}{2}}-(\sin^2\nu_2-\sin^2\nu_1\sin^2\nu_2)^{\frac{1}{2}}}{(1-\sin^2\nu_1-\sin^2\nu_2+\sin^2\nu_1\sin^2\nu_2)^{\frac{1}{2}}}\right]+l.$$

Now since α is small

$$\sin^2\nu_1=\sin^2\nu+2\alpha\sin\nu\cos\mu$$
$$\sin^2\nu_2=\sin^2\nu-2\alpha\sin\nu\cos\mu$$
$$\sin^2\nu_1\sin^2\nu_2=\sin^4\nu$$

$$\mathfrak{L}=\frac{r_1}{\cos^2\nu}\left[(\sin^2\nu-\sin^4\nu+2\alpha\sin\nu\cos\mu)^{\frac{1}{2}}-(\sin^2\nu-\sin^4\nu-2\alpha\sin\nu\cos\mu)^{\frac{1}{2}}\right]+l$$

$$=\frac{r_1\sin\nu}{\cos\nu}\left[\left(1+\frac{2\alpha\cos\mu}{\sin\nu\cos^2\nu}\right)^{\frac{1}{2}}-\left(1-\frac{2\alpha\cos\mu}{\sin\nu\cos^2\nu}\right)^{\frac{1}{2}}\right]+l\ .$$

But if x is small $(1+x)^{\frac{1}{2}}=1+x/2$

$$\mathfrak{L}=2r_1\alpha\cos\mu/\cos^3\nu+l \tag{1}$$

$$=2\alpha\sec\mu\left[\frac{r_1\cos^2\mu}{[1-(\zeta+\sin\mu)^3]^{3/2}}+r_0\right] \tag{2}$$

$$=2\alpha\sec\mu[r_1\cos^2\mu/\cos^3\nu+r_0]\ . \tag{3}$$

For the normal-beam method ($\mu=0$) this reduces to equation (22) of Phillips (1954).

For the equi-inclination method ($\sin\mu=-\zeta/2=-\sin\nu$) equation (1) becomes

$$\mathfrak{L}=2r_1\alpha/\cos^2\nu+l\quad\text{where}\quad\cos^2\nu=(1-\zeta^2/4)$$

which is ($\sec\nu$) times equation (26) of Phillips (1954).

† *Notes* (1) r_0 may have to be determined experimentally by taking photographs on the same film in (stationary) cameras of different radii, but with the same collimator system; or by measuring the variation of spot size in a specially designed film pack. The 'source' is not necessarily coincident with the collimator pinhole. The value of r_0 is important and must not be assumed.

(2) Phillips (1954) gives $l=2\alpha\mathfrak{R}_2$; but this only applies in the normal-beam method.

Calculation of angular range of reflexion, $\Delta\varphi$

Following Phillips, $\Delta\varphi=(\cos\varphi_1-\cos\varphi_2)/\sin\varphi$ when $\Delta\varphi$ is small.

From equation (3), p. 176 of *I.T.* Vol. II

$$\cos\varphi=\frac{\zeta^2+\xi^2+2\zeta\sin\mu}{2\xi\cos\mu}\quad\text{where}\quad\zeta^2+\xi^2=4\sin^2\theta=d^{*2}$$

$$\sin\varphi=\frac{1}{2\xi\cos\mu}[4\xi^2\cos^2\mu-4\zeta^2\sin^2\mu-(\zeta^2+\xi^2)(\zeta^2+\xi^2+4\zeta\sin\mu)]^{\frac{1}{2}}$$

$$=\frac{1}{2\xi\cos\mu}[d^{*2}(4\cos^2\mu-4\zeta\sin\mu-d^{*2})-4\zeta^2]^{\frac{1}{2}}$$

$$\cos\varphi_1=\frac{\zeta^2+\xi^2+2\zeta\sin(\mu+\alpha)}{2\xi\cos(\mu+\alpha)}=\frac{d^{*2}+2\zeta\sin A}{2\xi\cos A}$$

$$\cos\varphi_2=\frac{\zeta^2+\xi^2+2\zeta\sin(\mu-\alpha)}{2\xi\cos(\mu-\alpha)}=\frac{d^{*2}+2\zeta\sin B}{2\xi\cos B}$$

$$\Delta\varphi=\frac{d^{*2}(\cos B-\cos A)+2\zeta(\sin A\cos B-\sin B\cos A)}{2\xi\cos A\cos B\sin\varphi}$$

$$=\frac{2d^{*2}\sin\frac{1}{2}(A+B)\sin\frac{1}{2}(A-B)+2\zeta\sin(A-B)}{\xi[\cos(A+B)+\cos(A-B)]\sin\varphi}$$

$$=2\frac{d^{*2}\sin\mu\sin\alpha+\zeta\sin2\alpha}{\xi(\cos2\mu+\cos2\alpha)\sin\varphi}$$

$$=2\alpha\frac{d^{*2}\sin\mu+2\zeta}{2\xi\cos^2\mu\sin\varphi}\quad\text{since }\alpha\text{ is small}$$

$$=2\alpha\frac{\sec\mu[d^{*2}\sin\mu+2\zeta]}{[d^{*2}(4\cos^2\mu-4\zeta\sin\mu-d^{*2})-4\zeta^2]^{\frac{1}{2}}} \tag{4}$$

$$=2\alpha\frac{\sec\mu[(\zeta^2+\xi^2)\sin\mu+2\zeta]}{[(\zeta^2+\xi^2)(4\cos^2\mu-4\zeta\sin\mu-\zeta^2-\xi^2)-4\zeta^2]^{\frac{1}{2}}}\ . \tag{5}$$

For the normal-beam method, this reduces to Phillips's (1954) equation (8); for the equi-inclination method, it reduces to

$$\Delta\varphi=\frac{\alpha\zeta}{\xi}[4-(\zeta^2+\xi^2)]^{\frac{1}{2}}\sec\mu=2\alpha\frac{\zeta}{\xi}\frac{\cos\theta}{\cos\nu}$$

which is ($\sec\mu$) times Phillips's (1954) equation (18).

Reflexion-spot length with camera translation

Taking the instrument constant C_2 of the Weissenberg camera as 2 when $\mathfrak{L}$ is measured in millimetres and φ in degrees, $\Delta\mathfrak{L}=\Delta\varphi/2$.

Hence

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{2\pi}\frac{\Delta\varphi}{\mathfrak{L}}=1\pm\frac{180}{2\pi}$$

$$\times\frac{(d^{*2}\sin\mu+2\zeta)[1-(\zeta+\sin\mu)^2]^{3/2}}{[d^{*2}(4\cos^2\mu-4\zeta\sin\mu-d^{*2})-4\zeta^2]^{\frac{1}{2}}[r_1\cos^2\mu+r_0[1-(\zeta+\sin\mu)^2]^{3/2}]}\ . \tag{6}$$

Since $d^{*2}=4\sin^2\theta$ and $\zeta=\sin\nu-\sin\mu$ this expression may also be written as

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{2\pi}$$

$$\times\frac{[(2\sin^2\theta-1)\sin\mu+\sin\nu]\cos^3\nu}{[4\sin^2\theta(\cos^2\theta-\sin\nu\sin\mu)-(\sin\nu-\sin\mu)^2]^{\frac{1}{2}}(r_1\cos^2\mu+r_0\cos^3\nu)}\ . \tag{7}$$

For upper layers of the *normal-beam setting* ($\mu=0$) formula (6) becomes

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{\pi}\frac{\zeta(1-\zeta^2)^{3/2}}{[4\xi^2-(\zeta^2+\xi^2)^2]^{\frac{1}{2}}[r_1+r_0(1-\zeta^2)^{3/2}]}$$

which is Phillips's equation (29), so that the ordinary normal-beam charts can be used with ζ and ξ referred to the $K\beta$ reflexions. Or, in terms of ν and θ

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{2\pi}\frac{\sin\nu\cos^3\nu}{(4\sin^2\theta\cos^2\theta-\sin^2\nu)^{\frac{1}{2}}(r_1+r_0\cos^3\nu)}\,. \tag{8}$$

When $\mu=-\nu$ (*equi-inclination setting*), then $\zeta=2\sin\nu=-2\sin\mu$ and the expression (6) becomes

$$\begin{aligned}\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}&=1\pm\frac{180}{4\pi}\frac{[4\zeta-\zeta(\zeta^2+\xi^2)](1-\frac{1}{4}\zeta^2)^{3/2}}{[(\zeta^2+\xi^2)(4-\xi^2)-4\zeta^2]^{\frac{1}{2}}\times[r_1(1-\frac{1}{4}\zeta^2)+r_0(1-\frac{1}{4}\zeta^2)^{3/2}]}\\&=1\pm\frac{180}{4\pi}\frac{\zeta(4-\zeta^2-\xi^2)(1-\frac{1}{4}\zeta^2)^{\frac{1}{2}}}{(4\xi^2-\xi^2\zeta^2-\xi^4)^{\frac{1}{2}}[r_1+r_0(1-\frac{1}{4}\zeta^2)^{\frac{1}{2}}]}\\&=1\pm\frac{180}{4\pi}\frac{\zeta(4-\zeta^2)^{\frac{1}{2}}(4-\zeta^2-\xi^2)^{\frac{1}{2}}}{\xi[2r_1+r_0(4-\zeta^2)^{\frac{1}{2}}]}\,.\end{aligned}$$

This expression, which is equivalent to that of Phillips's equation (30), is rather simpler in terms of ν and θ

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{2\pi}\frac{\sin\nu\cos\nu\cos\theta}{(\cos^2\nu-\cos^2\theta)^{\frac{1}{2}}(r_1+r_0\cos\nu)}\,. \tag{9}$$

Summary of formulae for upper-layer spot extension or contraction for Weissenberg camera radius r_1, constant $C_2=2$: camera axis parallel to axis of crystal rotation and source-to-crystal distance r_0

General case

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{2\pi}\frac{\cos^3\nu\,(\sin\nu-\cos 2\theta\sin\mu)}{[4\sin^2\theta\,(\cos^2\theta-\sin\nu\sin\mu)-(\sin\nu-\sin\mu)^2]^{\frac{1}{2}}(r_1\cos^2\mu+r_0\cos^3\nu)}\,.$$

Normal-beam setting

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{2\pi}\frac{\sin\nu\cos^3\nu}{(\cos^2\nu-\cos^2 2\theta)^{\frac{1}{2}}(r_1+r_0\cos^3\nu)}\,.$$

Equi-inclination setting

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{2\pi}\frac{\sin\nu\cos\nu\cos\theta}{(\cos^2\nu-\cos^2\theta)^{\frac{1}{2}}(r_1+r_0\cos\nu)}\,.$$

Anti-equi-inclination setting

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{2\pi}\frac{\sin\nu\cos\nu\sin\theta}{(\cos^2\nu-\sin^2\theta)^{\frac{1}{2}}(r_1+r_0\cos\nu)}\,.$$

Flat-cone setting

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{2\pi}\frac{\sin\mu\cos 2\theta}{(\cos^2\mu-\cos^2 2\theta)^{\frac{1}{2}}(r_1\cos^2\mu+r_0)}\,.$$

In all cases the correction may be applied by combining it with the Lorentz correction which in each case may be expressed as follows:

General case

$$L^{-1}=\cos\nu\cos\mu\sin\Upsilon$$

where

$$\cos\Upsilon=\frac{\cos^2\nu+\cos^2\mu-\xi^2}{2\cos\nu\cos\mu}$$

$$\xi^2=4\sin^2\theta-(\sin\nu-\sin\mu)^2$$

from equations (1), (2), (4) of section 4.3.2.1 of *I.T.* Vol. II.

Hence

$$L^{-1}=[4\sin^2\theta\,(\cos^2\theta-\sin\nu\sin\mu)-(\sin\nu-\sin\mu)^2]^{\frac{1}{2}}$$

and

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{2\pi}\frac{L\cos^3\nu\,(\sin\nu-\sin\mu\cos 2\theta)}{(r_1\cos^2\mu+r_0\cos^3\nu)}\,.$$

Normal-beam setting

$$L^{-1}=(\sin^2 2\theta-\zeta^2)^{\frac{1}{2}}=(\cos^2\nu-\cos^2 2\theta)^{\frac{1}{2}}$$

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{2\pi}\frac{L\sin\nu\cos^3\nu}{r_1+r_0\cos^3\nu}\,.$$

Equi-inclination setting

$$L^{-1}=2\cos\theta\,(\cos^2\nu-\cos^2\theta)^{\frac{1}{2}}$$

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{\pi}\frac{L\cos\nu\sin\nu\cos^2\theta}{r_1+r_0\cos\nu}\,.$$

Anti-equi-inclination setting

$$L^{-1}=2\sin\theta\,(\cos^2\nu-\sin^2\theta)^{\frac{1}{2}}$$

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{\pi}\frac{L\cos\nu\sin\nu\sin^2\theta}{r_1+r_0\cos\nu}\,.$$

Flat-cone setting

$$L^{-1}=(\cos^2\mu-\cos^2 2\theta)^{\frac{1}{2}}$$

$$\frac{\mathfrak{L}\pm\Delta\mathfrak{L}}{\mathfrak{L}}=1\pm\frac{180}{2\pi}\frac{L\cos 2\theta\sin\mu}{r_1\cos^2\mu+r_0}\,.$$

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