HELMHOLTZ, L. (1936). *J. Chem. Phys.* **4**, 316.
Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935). Berlin: Borntraeger.
JAMES, R. W. (1948). *The Crystalline State*, vol. 2, appendix 3. London: Bell.
MATHIESON, A. McL. (1952). *Acta Cryst.* **5**, 332.
PAULING, L. (1940). *The Nature of the Chemical Bond.* Ithaca: Cornell University Press.
PEERDEMAN, A. F., BOMMEL, A. J. VAN & BIJVOET, J. M. (1951). *Proc. Acad. Sci. Amst.* **54**, 16.

Acta Cryst. (1954). **7**, 709

A Theoretical Possibility of Correcting the Collimation Error in Small-Angle X-ray Scattering

BY KATARINA KRANJC

Physical Institute, Faculty of Science, University of Zagreb, Zagreb, Yugoslavia

(*Received* 25 *May* 1954 *and in revised form* 5 *July* 1954)

A general solution for correcting the collimation error in small-angle X-ray scattering is considered. The experimentally obtained intensity function can be expressed analytically as the convolution of the correct intensity function and the intensity distribution on the trace of the primary beam in the film. The correction of the experimental scattering curve is possible by using the convolution theorem for multiple Fourier transforms.

The effect of imperfect collimation of the primary beam on the angular intensity distribution of scattered radiation at small angles is called collimation error (Yudowitch, 1949*a*). Several authors have studied the possibility of correcting the experimentally obtained scattering curve (Jellinek & Fankuchen, 1945; Guinier & Fournet, 1947; DuMond, 1947; Shull & Roess, 1947; Franklin, 1950; Kratky, Porod & Kahovec, 1951). It was shown that the correction is possible only assuming that certain properties are attributed to the energy distribution in the primary beam, or to the shape of the beam-defining apertures, or to the shape of the scattering function. Yudowitch (1949*a*, *b*, 1952) investigated the geometrical conditions of the collimating system under which the collimation error may be reduced to its minimum.

Hosemann (1951) gave a general formula expressing the relationship between the experimental scattering function I and the correct function I_0; the latter would be obtainable if an incident parallel beam of infinitely small cross section were available. This formula does not imply any assumption of the energy distribution in the primary beam and of the shapes of the collimation apertures or of the shapes of scattering curves. The aim of this paper is to show that the correcting of experimental scattering function I is possible also in such a general case, using the convolution theorem for multiple Fourier transforms. The method to be described is analogous to the method of correcting the experimentally obtained line widths and shapes in Debye–Scherrer diagrams, proposed by Shull (1946) and applied by Stokes (1948). The difference between these two methods lies in the fact that the functions to be considered in the collimation-error problem are two-variable functions, while line-shape correcting could be regarded as a one-dimensional problem.

Let us deduce Hosemann's formula for the case of registering the small-angle scattering on a photographic film. The rectangle in Fig. 1 represents the trace

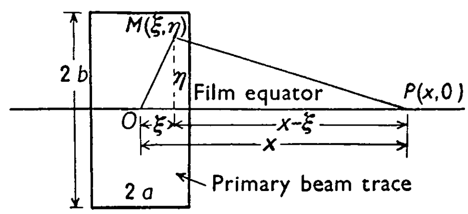

Fig. 1. See text for explanation.

of the primary beam on the film. We want to get the intensity of the scattered rays reaching the point $P(x, 0)$ on the film equator. A part of the energy of primary X-rays falling on the surface element $d\xi d\eta$ around the point M is scattered in the specimen towards the point P. The scattering angle of these rays is directly proportional to the distance MP. Thus the intensity of these scattered rays is proportional to $I_0(MP)$, or to $I_0(x-\xi, \eta)$. If we denote the intensity distribution function on the trace of the primary beam by $G(\xi, \eta)$, the contribution of the examined part of the incident beam to the intensity at point P is

$$dI = G(\xi, \eta) I_0(x-\xi, \eta) d\xi d\eta \,.$$

We obtain the whole intensity of radiation scattered towards the point P by integration over the area of the primary beam trace:

$$I(x) = \int_{-a}^{+a}\int_{-b}^{+b} G(\xi, \eta) I_0(x-\xi, \eta) d\xi d\eta \, , \qquad (1)$$

where the function G is to be normalized, i.e.

$$\int_{-a}^{+a}\int_{-b}^{+b} G(\xi, \eta) d\xi d\eta = 1 \, .$$

Now, we can express (1) in a more general form:

$$I(x, y) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} G(\xi, \eta) I_0(x-\xi, y-\eta) d\xi d\eta \, . \qquad (2)$$

The extension of the integration limits is allowable owing to the fact that I_0 falls rapidly to zero outside the range of small angles.

The function $I(x, y)$, as expressed by (2), is called the convolution, or *Faltung*, of the functions of two variables I_0 and G:

$$I(x, y) = G(x, y) * I_0(x, y) \, .$$

To express the function I_0 explicitly we shall use the convolution theorem which states that the Fourier transform of the convolution of two functions is the product of their Fourier transforms (see for instance Bochner & Chandrasekharan, 1949). Now, i, g and i_0 being the Fourier transforms of the functions I, G and I_0, defined by the relations

$$i(r, s) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} I(x, y) e^{i(rx+sy)} dx dy \, ,$$

$$g(r, s) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} G(x, y) e^{i(rx+sy)} dx dy \, ,$$

$$i_0(r, s) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} I_0(x, y) e^{i(rx+sy)} dx dy \, ,$$

the convolution theorem may be expressed as

$$i(r, s) = g(r, s) . i_0(r, s)$$

or

$$i_0(r, s) = i(r, s)/g(r, s) \, .$$

Applying the inversion theorem for multiple Fourier transforms, we obtain

$$I_0(x, y) = \frac{1}{4\pi^2}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} i_0(r, s) e^{-i(xr+ys)} dr ds \, .$$

Since we are interested in the special case of $y = 0$, we may write

$$I_0(x) = \frac{1}{4\pi^2}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} i_0(r, s) e^{-ixr} dr ds \, . \qquad (3)$$

Equation (3) is the general solution of the collimation-error problem. In principle, it makes possible the correction of the experimental scattering curve by numerical or graphical integration. The usual microphotometering of the diffraction pattern along the film equator gives the function $I(x)$. Since generally I is not a radially symmetric function, the function $I(x,y)$, i.e. the spatial intensity distribution of scattered radiation, must be determined from the diffraction pattern. It can be obtained by microphotometering the diffraction pattern in several rows, the number of which is determined by the requirements of numerical integration. Of course, the function thus obtained is to be extrapolated over the range of the primary beam trace. The function $G(x, y)$ can be deduced mathematically from the collimation geometry, or experimentally by microphotometering the trace of the primary beam; the trace can be obtained by exposing the bare film to primary X-rays for a short time. The latter method gives only the shape of the desired function; the real extent of the trace must be deduced from the geometrical conditions of the collimating system.

In the case of the pinhole-shaped beam-defining apertures, G and I are radially symmetric functions and thus the photometering along only one diameter is sufficient.

References

Bochner, S. & Chandrasekharan, K. (1949). *Fourier Transforms*, p. 58. Annals of Mathematics Studies, Number 19. Princeton: University Press.

DuMond, J. W. M. (1947). *Phys. Rev.* **72**, 83.

Franklin, R. E. (1950). *Acta Cryst.* **3**, 158.

Guinier, A. & Fournet, G. (1947). *J. Phys. Radium*, **8**, 345.

Hosemann, R. (1951). *Ergebn. exakt. Naturw.* **24**, 142.

Jellinek, M. H. & Fankuchen, I. (1945). *Industr. Engng. Chem.* **37**, 158.

Kratky, O., Porod, G. & Kahovec, L. (1951). *Z. Elektrochem.* **55**, 53.

Shull, C. G. (1946). *Phys. Rev.* **70**, 679.

Shull, C. G. & Roess, L. C. (1947). *J. Appl. Phys.* **18**, 295.

Stokes, A. R. (1948). *Proc. Phys. Soc.* **61**, 382.

Yudowitch, K. L. (1949*a*). *J. Appl. Phys.* **20**, 174.

Yudowitch, K. L. (1949*b*). *J. Appl. Phys.* **20**, 1232.

Yudowitch, K. L. (1952). *Rev. Sci. Instrum.* **23**, 83.