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References

DIAMOND, R. (1966). *Acta Cryst.* **21**, 253.
MAIN, P. & ROSSMANN, M. G. (1966). *Acta Cryst.* **21**, 67.
ROSSMANN, M. G. & BLOW, D. M. (1962). *Acta Cryst.* **15**, 24.
ROSSMANN, M. G. & BLOW, D. M. (1963). *Acta Cryst.* **16**, 39.
ROSSMANN, M. G. & BLOW, D. M. (1964). *Acta Cryst.* **17**, 1474.
ROSSMANN, M. G., BLOW, D. M., HARDING, M. M. & COLLER, E. (1964). *Acta Cryst.* **17**, 338.

Acta Cryst. (1967). **22**, 764

An Optical Instrument for the Direct Interpretation of Laue Patterns

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An optical apparatus is described for the direct interpretation of Laue photographs. It presents the results in the form of radial projections of the lattice-plane normals on a spherical surface.

For the interpretation of Laue patterns graphical methods are available which lead either to the gnomonic or to the stereographic projection. In order to eliminate the point-by-point plotting involved in these procedures, we have tried to find an optical method capable of yielding the required projection of a large area of the film simultaneously. Moreover, we aimed at a radial projection of the lattice plane normals on a spherical surface, because this allows direct recognition of symmetry elements even for arbitrary crystal settings. Such elements are, indeed, hard to find from the above-mentioned plane projections. On the other hand, the advantages of the latter (angle-true image by stereographic projection, easy recognition of zones by the gnomonic one) are obviously retained in full in the radial projection.

The basic idea of the resulting method is explained in Fig. 1. A Laue photograph (L) is placed before a point source (O), in such a way that the geometry of light source and film, while being projected, is exactly the same as the geometry of crystal and film while the latter was exposed. A light-ray going from O to a spot S on the film then corresponds to the X-ray pencil which caused this spot.

After passing the film, the light-ray is reflected at P by a curved mirror to a ground glass sphere, intersection Q. Upon this sphere, a distorted shadow projection of the film is formed. Now the distortion has to be such that the line OQ be perpendicular to the lattice-plane (V) which diffracted the X-rays in the direction OP.

The film is shown as a cylinder in Fig. 1, but it will be clear that any film shape can be used, provided the geometry of the film-holder of the optical apparatus is again identical with that of the X-ray camera.

It will be equally clear that the mirror shows rotational symmetry, with XO, which corresponds to the direction of the incident X-rays, as axis. The shape of the mirror-curve is not yet fixed by the condition imposed. The condition leaves one degree of freedom so that the axial plane contains an infinite number of curves

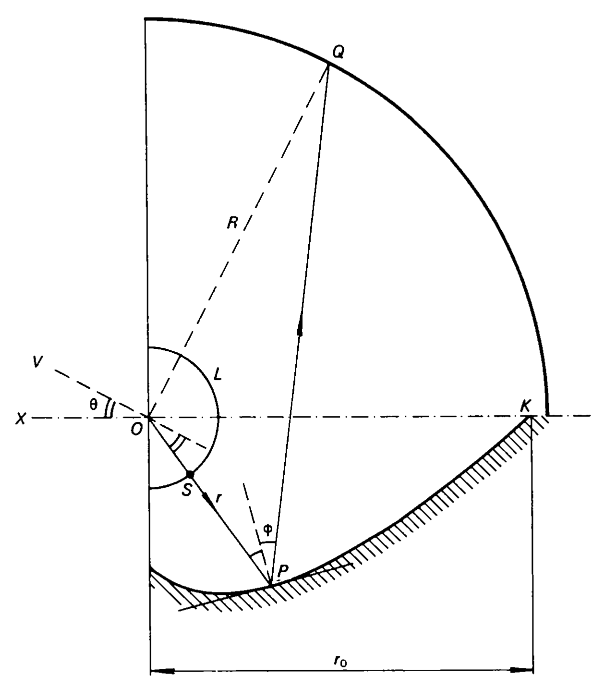

Fig. 1. Geometry of the instrument.

reflecting the light-ray to the point Q; we can distinguish them by the value of their axial length ($r_0 = OK$).

The equation of the mirror-curve follows from Fig. 2, which gives part of the mirror magnified. Putting $OP = r$, and calling θ the Bragg angle and φ the angle of incidence of the ray on the mirror, we observe that the differential equation for the curve is:

$$dr/d\theta = -2r \tan \varphi \,. \tag{1}$$

From Fig. 1 one derives

$$r = R\,(\cos \theta \cot 2\varphi - \sin \theta) \tag{2}$$

so that r can be eliminated from equation (1), yielding:

$$\frac{\tan^2\varphi + 1}{2 \tan^4\varphi}\,\frac{d(\tan \varphi)}{d\theta} + \frac{3 \tan^2\varphi + 1}{2 \tan^3\varphi} \tan \theta + 1 = 0 \,. \tag{3}$$

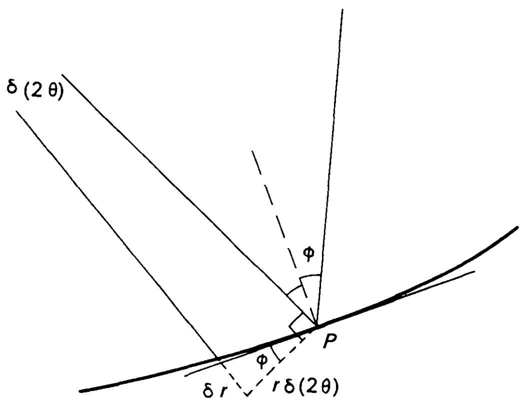

Fig. 2. Part of the mirror curve (schematic).

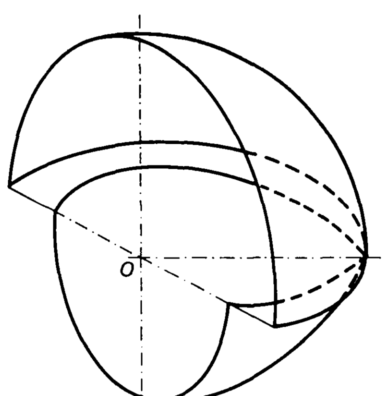

Fig. 3. Sketch of the instrument showing the separation of spherical shield and mirror by a plane. In this sketch, R is taken (arbitrarily) equal to r_0, just as in the prototype.

By trial and error one finds that multiplying (3) by $\cos^3\theta$ makes it an exact differential equation: $dF(\theta, \tan \varphi)/d\theta = 0$, the solution of which turns out to be

$$F(\theta, \tan \varphi) = -\cos^3\theta(3 \tan^2\varphi + 1)/6 \tan^3\varphi + \sin \theta - \tfrac{1}{3} \sin^3\theta = C \,. \tag{4}$$

The constant C is determined by the ratio r_0/R:

$$C = -(3 \tan^2\varphi_0 + 1)/6 \tan^3\varphi_0, \quad \text{wherein } \varphi_0 = \tfrac{1}{2} \tan^{-1}(R/r_0) \,. \tag{5}$$

Calling

$$\tfrac{1}{2} \cos^3\theta/(3 \sin \theta - \sin^3\theta - 3C) = f \tag{6}$$

in which f is a function of θ and r_0/R only, we can reduce (4) to

$$\tan^3\varphi - f(3 \tan^2\varphi + 1) = 0 \,. \tag{7}$$

The solution of this equation can be written down with the help of the formula of Cardan:

$$\tan \varphi = f + \{\tfrac{1}{2}f + f^3 + f(\tfrac{1}{4} + f^2)^{\frac{1}{2}}\}^{1/3} + \{\tfrac{1}{2}f + f^3 - f(\tfrac{1}{4} + f^2)^{\frac{1}{2}}\}^{1/3} \,. \tag{8}$$

Substitution of this result in (2) then gives the polar equation of the mirror curve.

This explicit solution of the problem is not written down here, because of the great length and complexity of the resulting formula. A numerical computation has to be made step by step, using (6), (8) and (2). With the help of a simple computer program we had 200 points of the curve computed in the θ-range from 0 to 90°.

It is very surprising that for (3) an integrating factor can be found which is a function of θ only. This suggests the existence of other variables which would show in a clear way the geometrical properties of the curve. Such variables have, however, not been found; nor does, for instance, the curvature reveal striking features.

For obvious geometrical reasons only half of the mirror and two octants of the sphere can be used, as shown in Fig. 3. A prototype of this instrument has been made, with $R = r_0 = 23{\cdot}2$ cm, the mirror covering the range from 1 to 90° in 2θ. In a dimmed light it yields very clear images when positive copies of Laue photographs are used. The point source was a 40× reduced image of a common 25W bulb obtained with a microscope objective, n.a. = 0·65. False light is effectively screened off by a slit along the axis in the plane which separates the sphere from the mirror (Fig. 3). The mirror was turned in brass on a copying lathe, using a steel template. It was silvered afterwards. The smoothness required comes close to optical criteria, especially with regard to long-range waviness.