Fig. 2, values of the argument for which the function becomes negative, can be found only after throwing over the hinged flap, which will change the colour presented by the whole scale.

Calculation proceeds along a line in the reciprocal lattice, e.g., by setting the two top scales at fixed values of $k.y_n$ and $l.z_n$, and reading the triple product from the bottom scale by running the cursor through all values of $h.x_n$. (A table of the multiples of the atomic coordinates has to be prepared prior to calculation.) Before the result is read, however, the scattering factor graph is adjusted to the appropriate value of $\sin^2\theta$ and the end mark of the bottom scale made to coincide with the curve, to include the scattering factor into the product. In the high symmetry systems in which triple product formulae occur, $\sin^2\theta$ is often of the form, $h^2A+k^2B+l^2C$, so that only values of, say, k^2B+l^2C need be tabulated in advance, the third term being added graphically as indicated in Fig. 1. (The use of a different function of θ in the f-graph, such as the cylindrical coordinates of the reciprocal lattice, may be preferable where values of it had to be calculated earlier—e.g., for Lorentz-polarization correction.)

With proper care, the device can be made accurate enough even for the more advanced stages of structure determinations. In a precision model, the body was made of plexiglass and reinforced by a hard aluminium alloy base plate. The scale carriers were made of the same alloy. The scales were hand drawn and reduced photographically onto aluminium offset foil, to eliminate the uneven shrinkage of the more conventional photographic media. Care was taken to check the trueness of the photographic apparatus, a printer's reducing machine. The scales were coated with protective varnish and fastened to their carriers with araldite cement. The stage for the f-graph must have a smooth movement, which can be achieved by letting it run on small tapered wheels in a V-groove machined into its base plate. The whole f-stage is detachable from the rest of the apparatus. For this model, the standard deviation of the triple product was found to be, in 100 trial multiplications, two units in the 1000 constituting the range of the product scale. In most cases, the uncertainty due to the temperature and atomic scattering factors will be greater than this.

An alternative possibility is to use blank cyclometric scales on which, by matching them against a master scale, only those values of $\cos hx_n$ or $\sin hx_n$ are marked that are actually needed; the index h, k or l is written down, and different colours are used for positive and negative values. In this way, the interpolations are made once for all, and large series of structure factors can be calculated in a shorter time. On the other hand, the accuracy may be somewhat lower, depending upon the care taken in drawing the ad-hoc scales.

The first model of this device was built in 1955, when both authors were guests at the Institute of Chemistry at Uppsala University. We wish to record our gratitude to Prof. G. Hägg for his permission to have a prototype built in the workshop of the Institute. We also gratefully acknowledge the grants that formed the basis of our sojourns at Uppsala: from Statens Naturvetenskapliga Forskningsråd—the Swedish Natural Science Research Council—(H. F.), and from Schweizerische Stiftung für Stipendien auf dem Gebiete der Mineralogie (A. N.).

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The effect of lattice imperfections on the interference function centroid.

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For a large perfect crystal, the interference function distribution in reciprocal lattice space is well known. The function has appreciable values only for positions very near reciprocal lattice points, and further the distribution is symmetric about each lattice point. As a result, the precise measurement of lattice parameters for crystals of high perfection is a relatively straight-forward procedure. For crystals containing a large number of imperfections, as in a cold worked metal, the interference function has appreciable values over a large region of reciprocal lattice space. Further there is no obvious relationship between the interference function distribution and the corresponding distribution of lattice strains in the crystal. Thus, if diffraction techniques are to be used to obtain precision parameter measurements for imperfect crystals, it is necessary to show that some property of the interference function can be used to define a mean lattice parameter. In this paper it is shown that the centroid of the interference function for the region surrounding the (h, k, l) reciprocal lattice point corresponds very nearly to the mean reciprocal (h, k, l) interplanar spacing.

We start by using a method similar to that developed by Warren & Averbach (1950) and Warren (1955). An imperfect crystal is considered in which the unit cells are displaced from their correct positions. The crystal axes (a, b, c) are chosen in a manner convenient for this problem. The c axis is taken to have a component normal to the (h, k, l) plane which is equal in length to the mean interplanar spacing and the other two axes are fixed in the (h, k, l) plane. In terms of these three axes, the position of any unit cell is given by

$$r_{uvw}=ua+vb+wc+ax_{uvw}+by_{uvw}+cz_{uvw}\,, \qquad (1)$$

where u, v, w are integers and x, y, z represent the displacement of the u, v, w unit cell from its regular position. It is assumed that the lattice strains in the deformed crystal are small; therefore, x, y, z are small compared to u, v, w respectively. The magnitudes and direction of a, b, c are fixed by the condition that

$$\bar{x}=\bar{y}=\bar{z}=0\,, \qquad (2)$$

where $\bar{x}$ is the mean value of x averaged over all u, v, w, and similar definitions apply to $\bar{y}$ and $\bar{z}$.

In terms of the crystal axes a, b, c it is possible to define reciprocal lattice axes a^*, b^*, c^* in the usual manner. If ξ, η, ζ represent variables along the a^*, b^*, c^* axes respectively, the interference function can be expressed in terms of these quantities. Warren has shown that with the particular choice of axes used, only the z displacement causes a broadening of the reciprocal lattice spot in the c^* direction. On integrating the interference function with respect to ξ, and η, the functional dependence on ζ only is obtained. Warren derived the following equation for this case.

$$I_0(\zeta) = N \sum_{n=0}^{\infty} A_n \cos 2\pi n\zeta + B_n \sin 2\pi n\zeta \,, \tag{3}$$

where ζ is defined so that ζc^* represents a distance along the c^* axis from the (h, k, l) reciprocal lattice point, and

$$A_o = N_3 \tag{4}$$

$$A_n = 2 \sum_{w=0}^{N_3} \cos 2\pi(z_w - z_{w+n}) \tag{5}$$

$$B_o = 0 \tag{6}$$

$$B_n = 2 \sum_{w=0}^{N_3} \sin 2\pi(z_w - z_{w+n}) \,, \tag{7}$$

where N_3 is the number of unit cells in the crystal in the c direction, N is the number of unit cells contained in a single reflecting plane, and the summation is taken over any column of unit cells defined by u and v equal to constants.

The deviation of the centroid position of the interference function from the reciprocal lattice point is given by

$$\bar{\zeta} = \frac{\int_{-\frac{1}{2}}^{\frac{1}{2}} \sum_{n=0}^{\infty} (A_n \cos 2\pi n\zeta + B_n \sin 2\pi n\zeta)\zeta \, d\zeta}{\int_{-\frac{1}{2}}^{\frac{1}{2}} \sum_{n=0}^{\infty} (A_n \cos 2\pi n\zeta + B_n \sin 2\pi n\zeta) \, d\zeta} \,. \tag{8}$$

Evaluation of equation (8) results in

$$\bar{\zeta} = \sum_{n=1}^{\infty} [(-1)^n / 2\pi n] B_n \,. \tag{9}$$

From equation (9) it would appear that $\bar{\zeta}$ is zero only for certain types of imperfect lattices, the most obvious being a lattice where positive and negative strains of the same magnitude are equally probable. Because, even for strains sufficiently small to have a good probability of existing in a cold worked metal, the elastic modulii depend on strain amplitude; the exact satisfaction of this type of strain distribution is not obvious. However, under certain quite general conditions it will be shown that the series of equation (9) converges to negligibly small values.

From equation (7) it follows that

$$B_1 = 2N_3\{ -[(2\pi)^3/3!]\overline{\Delta z_1^3} + [(2\pi)^5/5!]\overline{\Delta z_1^5} - \ldots \} \,, \tag{10}$$

where

$$\overline{\Delta z_1^3} = (1/N_3) \sum_{n=0}^{N_3} (z_n - z_{1+n})^3 .$$

From equation (3) it follows that

$$B_1 = (2/N) \int_{-\frac{1}{2}}^{\frac{1}{2}} I_0(\zeta)[2\pi\zeta - (2\pi\zeta)^3/3! + (2\pi\zeta)^5/5! - \ldots] d\zeta \,. \tag{11}$$

Combining equations (10) and (11) we find

$$2\pi\bar{\zeta} = [(2\pi)^3/3!][\overline{\zeta^3} - \overline{\Delta z_1^3}] - [(2\pi)^5/5!][\overline{\zeta^5} - \overline{\Delta z_1^5}] + \ldots . \tag{12}$$

If the interference function decreases to zero sufficiently rapidly as ζ increases, the third and all higher moments of the distribution are very small. Similarly, if the lattice strains between neighboring unit cells are sufficiently small, the higher moments of the strain distribution are negligible. Under these conditions $\bar{\zeta}$ is very nearly zero.

If we make the reasonable assumption that $\overline{\zeta^3}$ and $\overline{\Delta z_1^3}$ are both of the same order; an estimate of $\bar{\zeta}$ can be obtained for typical cold worked metals. For example, if we take $2 \cdot 10^{-3}$ as an upper limit for both $(\overline{\zeta^3})^{\frac{1}{3}}$ and $(\overline{\Delta z_1^3})^{\frac{1}{3}}$, then $\bar{\zeta} < 10^{-7}$, certainly a value which can be neglected.* Thus the percentage error introduced by approximating the reciprocal mean interplanar spacing by the position of the interference function centroid is about of the same order as the mean cubed strain between neighboring unit cells.

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* These values seem conservative, since by use of the Warren & Averbach analysis $(\overline{\Delta z_1^3})^{\frac{1}{3}}$, it is found to be of the order 10^{-2} to 10^{-3} for cold worked metals (Hirsch, 1956). The third moment should be much lower, of course, since positive and negative strains would partially cancel.

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A note on the heavy-atom method.

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In a recent paper (Sim, 1959) on the application of the heavy-atom method to non-centrosymmetric structures it was shown that improved resolution of the atoms could be obtained by employing in the Fourier series calculated from the phase angles α_H, amplitudes $W|F|$ rather than $|F|$, the weight W assigned to any term depending on the probable magnitude of the phase-angle error $(\alpha - \alpha_H)$. As the electron-density distribution is fairly insensitive to the precise set of weights adopted, any weighting function which increases smoothly from 0 to 1 as