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Two aids for the calculation of crystal structure factors.

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In this institute two devices have been found to be very useful for the calculation of structure factors and similar functions (determination of phase angles, calculation of the series in differential synthesis). The first of these devices (I) facilitates the calculation of the angles $\phi = hx + ky + lz$ for each atom with the co-ordinates (x, y, z), where ϕ, x, y and z are expressed in millicycles $(= 2\pi/1000)$. The second device (II) facilitates the calculation of $f\left\{\frac{\sin}{\cos}\right\}\phi$.

I. With an ordinary multiplying machine the calculation of ϕ is most rapidly carried out by keeping two indices constant and entering the sum of the two corresponding terms in the result-register. The third parameter is then entered in the setting board and ϕ obtained for each value of the third index without any change in setting. A multiplying machine can, however, be rather easily changed so that it permits the variation of two or three indices without any change in setting. The possibility of a variation of two indices (I*a*) often means a considerable gain in speed while the additional gain of a variation of the third index (I*b*) is not so marked.

(*a*) A machine which makes the variation of two indices possible, has been obtained by slight changes of a Model 29 Original-Odhner machine (A.-B. Original-Odhner, Gothenburg, Sweden). This machine has a setting board with 10 levers. One of the parameters x, y, or z is set on the levers 1–3 (all numbering starting from the right), another on the levers 5–7. The levers 4, and 8–10 are cut off. The values of the two corresponding indices are read in the multiplier register on the dials 5, 6, and the dials 1, 2 respectively. The other dials are covered. The multiplier register has tens transmission, but this is broken between 2 and 3 by filing off the cam on dial 2 which actuates the transmission. If the first turn of the crank is positive, negative values of the indices will show as their complements to 100. The indication will then be unambiguous up to absolute index values of 49, which is sufficient for most purposes. The tens transmission enables short-cut multiplication.

With the above positions of the figures of parameters and indices the three last figures of the ϕ values will appear on the dials 5–7 of the result-register. As only these three figures are wanted, all other dials are covered. They are also put out of operation by removing the teeth of the wheels which act upon them. This can be done by twisting the teeth with a pair of pliers.

All these changes can be accomplished in any workshop in about an hour and the result will be a very useful machine.

(*b*) If the possibility of short-cut multiplication is desirable, there must be an inactive disk between two different parameter groups of the setting board. With parameter groups of three figures a machine which permits the variation of three indices will then require a drum of eleven disks, of which nos. 4 and 8 are inactive. Furthermore, the original multiplier register must have at least ten dials, of which six are to be active. This prevents the use of the Model 29 machine, whose multiplier register has only eight dials. The Model 24 Original-Odhner machine, however, which has a multiplier register with eleven dials, is suitable for this purpose and one such machine has been changed in this laboratory. The drum was extended by translating the disks 8, 9 and 10 one step to the left and inserting a blind dial in the place of no. 8. An extra slot for the setting lever of the disk with the new number 11 was cut in the shielding plate. The extension of the drum necessitated some additional but rather small changes in order to permit the function of the different blocking mechanisms. The other changes correspond to the ones mentioned under I(*a*).

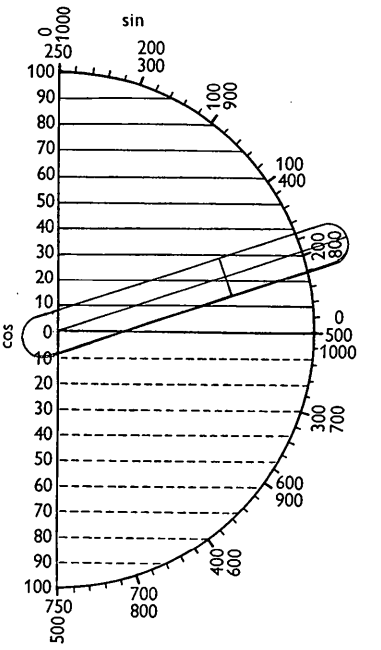

Fig. 1. Device for calculating $f\left\{\frac{\sin}{\cos}\right\}\phi$.

II. The calculation of $f\left\{\frac{\sin}{\cos}\right\}\phi$ is made graphically by means of the device schematically shown in Fig. 1. In order to reduce the dimensions only a semicircle is used. This is best drawn on parallel-ruled paper or, for lack of that, on square-ruled paper. An interval (chosen as unit) of 2·5 mm. between the lines is convenient, giving a radius of the circle of 250 mm. Every fifth line is inked, every tenth more heavily (only these last ones are drawn in Fig. 1). The inking in the positive half is in black and in the negative half in red (broken lines in Fig. 1). The semicircle is used in the position of Fig. 1 for reading sine values and turned 90° from this for reading cosine values. The corresponding ϕ values in millicycles are written along the circumference. The paper is mounted on a board and covered with a sheet of celluloid. A perspex ruler moves around the centre of the circle, and along the lower surface of the ruler a slider with a cross-mark can be translated. The ruler is first placed parallel to the

diameter and the cross-mark of the slider is set at the given value of f. The further procedure is obvious.

The combination I(a)+II does the same work as the machine devised by Evans & Peiser (1942). A disadvantage in comparison with that machine is that the computation is effected in two stages. On the other hand, the accuracy is much greater, and the speed of the operations is so high that it is doubtful whether the total time of computation will be larger. Owing to the low price of the small calculating machines used, the whole arrangement will be cheap.

Reference

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The shape transform in electron diffraction by small crystals.

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In considering the diffraction of X-rays or electrons by a small crystal the reciprocal lattice cannot be regarded simply as a lattice of points of extent negligible compared with the dimensions of the reciprocal cell, but one must take into account the finite extent of the crystal and the shape of its boundary. This was first discussed in detail by v. Laue (1936), who demonstrated that, as a result, the scattering amplitude about each reciprocal-lattice point would be extended in directions normal to the boundary faces of the crystals. Ewald (1940) and Patterson (1939) have refined v. Laue's treatment by considering the reciprocal lattice as the Fourier transform of the density distribution in the crystal. This was conveniently expressed mathematically by the use of a shape function $s(u_i)$ of the co-ordinates u_i, having the value 1 inside, and 0 outside, the crystal boundary. If $\rho(u_i)$ is the density distribution in the finite crystal and $\rho_\infty(u_i)$ that in the perfectly periodic infinite crystal, then

$$\rho(u_i)=\rho_\infty(u_i)\, s(u_i).$$

The Fourier transform $S(\xi_i)$ of the shape function $s(u_i)$, expressed as a function of the reciprocal-space co-ordinates ξ_i, then determines the distribution of scattering amplitude around each reciprocal-lattice integer point. Patterson (1939) has calculated the shape transform for a number of regular polyhedra. Their form around each reciprocal-lattice integral point is characterized by a principal maximum centred on the point and subsidiary maxima whose magnitude and position are determined by the size and shape of the crystal.

Using a high-resolution electron-diffraction camera designed and constructed in this laboratory (Cowley & Rees, unpublished), we have succeeded in demonstrating the existence of these subsidiary maxima in the individual reflexions from small ZnO particles. These may be seen in the reproductions of individual reflexions on the $11\bar{2}0$ ring in Figs. 1 and 2. To our knowledge, no authentic experimental proof of the existence of subsidiary maxima, and therefore of the complete optical theory of electron diffraction, has previously been obtained. The particles of ZnO prepared by burning the metal in air are known from electron microscopy to be needles of diameter 100–500 A. considerably elongated along [0001]; independent evidence from the refraction fine-structure in the same patterns (Rees & Spink, in preparation) suggests that these particles are either circular cylinders or hexagonal prisms with somewhat rounded edges. The shape transforms will therefore extend appreciably only in the reciprocal-lattice plane normal to c^*, and the resulting diffractions will be streaked at angles determined by the orientation of the crystal with respect to the beam and the indices of the particular reflexion.

We have derived the shape transform (for the elongated hexagonal prism) along two relevant directions. For the $[1\bar{1}00]$ direction it is of the form

$$\frac{4}{3}\left[\frac{\sin p}{p}+\frac{1-\cos p}{p^2}\right],$$

and for $[1\bar{1}20]$, $\dfrac{4}{3}\left[\dfrac{\cos q-2\cos^2 q+1}{q^2}\right]$.

Examination of these two functions shows that the complete transform will have extensions of largest amplitude along the directions $[1\bar{1}00]$, $[10\bar{1}0]$ and $[01\bar{1}0]$ from each integer point of the reciprocal lattice; along other directions (e.g. $[11\bar{2}0]$) the subsidiary maxima will decrease in amplitude very rapidly with distance from the integer point. For the circular cylinder, Patterson (1939) has shown that the shape transform is of the form $2J_1(p)/p$ for the direction $[h,k,\bar{h}+\bar{k},0]$, where $J_1(p)$ is the first-order Bessel function. For the elongated cylinder the transform may be pictured as a family of concentric tores lying in a plane normal to c^*. The properties of these transforms (for example, the positions of the maxima and zeroes) may be used to distinguish between the two possible crystal habits; also the separation of the subsidiary maxima may be used to obtain the crystal dimensions. The greatest diameter of the needle giving the reflexion indicated by the arrow in Fig. 1 is calculated to be 400 A., a value consistent with electron-microscopic observation. Moreover, the spacings of the maxima and zeroes suggest that this crystal at least has a hexagonal rather than circular section.

The intensity distribution illustrated in Fig. 2 shows a pair of broad maxima symmetrically disposed about the Bragg position and distinct from the structure associated with the shape transform. This is the result of refraction of the electron beam passing through a crystal of hexagonal section. The coexistence of refraction and interference effects in the fine structure of these patterns complicates their interpretation, but leads one to expect that for cylindrical crystals the subsidiary maxima would be obscured, except for extremely narrow crystals having negligible absorption.

A small improvement in resolution will permit the use of electron diffraction for the unambiguous determination