factors. This can be explained by the fact that the number of equations in A equals the number of structure factors, while in B this number equals the number of zero points. This might be important in practice with regard to the necessary computer time.

This note should conclude with some more general remarks. As methods A and B are based on different physical principles, it might be worth while to use both methods in centrosymmetrical structures in parallel, or to combine them. Furthermore, the distinguishing features of the methods in comparison with the squaring methods should be emphasized. There is no restriction whatsoever on the shape of the electron-density functions. There may be overlap (in projections), different weights of the atoms, *etc.* The last remark concerns the philosophy behind the methods. They have some common features with the heavy-atom and image-seekind methods in spite of their otherwise fundamental physical difference. All three techniques are based on certain information which first has to be extracted from the Patterson function. This information consists of the heavy-atom–heavy-atom peak in the heavy-atom technique, of the positions of single-weight Patterson peaks in the image-seeking methods, or, in the third case, of the positions of Patterson zero points in the methods discussed in this note. There is, however, one essential point in favour of the new methods. It is well known that it is sometimes very difficult to extract the necessary Patterson information for the initial steps of the first two methods. On the other hand, it is quite easy to find zero regions in a Patterson map or to use a simple computer program in connection with the phase-determining procedure.

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On minimum receiving apertures in single crystal diffractometry.

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In conjunction with a study of systematic errors in integrated intensity measurements (Ladell & Spielberg, 1963), we have derived the minimum dimensions of the receiving aperture required for both the 2:1 and ω-scan methods for crystals of circular cross section. A derivation of the minimum dimensions of the receiving aperture has already been reported by Alexander and Smith (1962) in a similar study, but our results for the case of a point source of monochromatic radiation incident upon a 'perfect' crystal of circular aperture do not agree with those reported. This case is of theoretical importance because (unlike the case of a crystal of negligible size) the requisite minimum aperture is a function of θ, the Bragg angle. Any attempt to evaluate the systematic error due to the use of a receiving aperture less than the minimum dimension must take this θ dependence into account.

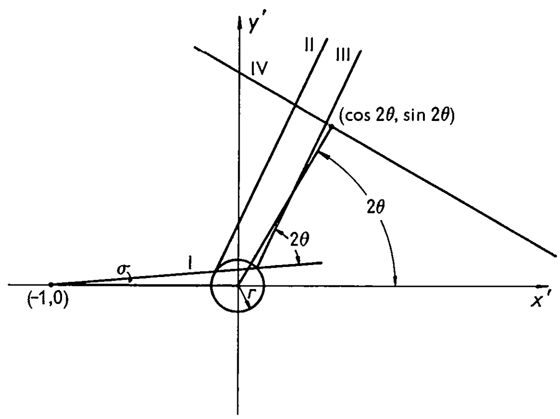

Fig. 1. Schematic of geometric construction used to derive the dimensions of minimum receiving apertures.

We place our crystal of radius r (Fig. 1) at the origin of a Cartesian coordinate system (designated $X'Y'$) and the point source at the coordinates $(-1, 0)$. Let σ measure deviation from the Bragg angle θ as the crystal is rotated counterclockwise. When $\sigma = 0$ diffraction takes place all along the diameter of the circular cross section which is collinear with the X' axis and the central diffracted ray is shown terminating at the coordinates $(\cos 2\theta, \sin 2\theta)$, at which point we place the center of the receiving aperture of the detector. When the crystal is rotated through an angle σ, an incident beam from $(-1, 0)$ proceeds along line I. Diffraction takes place along the chord formed by the part of line I intercepted by the circular cross section; the leading edge of the diffracted beam is denoted by line II and the trailing edge of the beam is denoted by line III. Line IV is normal to the central diffracted ray passing through $(\cos 2\theta, \sin 2\theta)$ and coincides with the trace of the detector in the plane of the drawing. In this derivation, for simplicity, the detector and point source are equidistant from the crystal. (The same analytic method can be employed to consider the case of unequal distances).

Lines II and III intersect line IV at points which are at displacements $s(\sigma)$ and $t(\sigma)$ from $(\cos 2\theta, \sin 2\theta)$, respectively. $|s(\sigma)|$ is a maximum for some positive value of σ and $t(\sigma)$ is a maximum for some negative value of σ. The required minimum aperture for the ω scan is $(|s(\sigma)|)_{\max} + (t(\sigma))_{\max}$. To find the width of the diffracted beam we must first find the explicit dependence of $s(\sigma)$ and $t(\sigma)$ upon σ. The derivation is as follows. We find the points of intersection of line I, $y' = (x'+1)\tan\sigma$, with the circle $x'^2 + y'^2 = r^2$. Since lines II and III which also pass through these points have tho slope $\tan(2\theta+\sigma)$ we can immediately write the equations of lines II and III. These are:

$$\frac{y' - \sin\sigma\{\cos\sigma \pm \sqrt{(r^2 - \sin^2\sigma)}\}}{x' + \sin^2\sigma \mp \cos\sigma\sqrt{(r^2 - \sin^2\sigma)}} = \tan(2\theta+\sigma)\,. \quad (1)$$

We now find the points of intersection of lines II and III with line IV whose equation is

$$\frac{y' - \sin 2\theta}{x' - \cos 2\theta} = -\cot 2\theta\,. \quad (2)$$

The displacement of these two points from $(\cos 2\theta, \sin 2\theta)$ are $s(\sigma)$ and $t(\sigma)$, respectively. The coordinates of the intersections of lines II and III with line IV having been found (solving for the simultaneous solutions of equations (1) and (2)), it is convenient to express these coordinates with reference to a new set of axes (XY) which is rotated $(2\theta - 90°)$ from the original set of axes $(X'Y')$. Using the equations of transformation,

$$\begin{aligned} x &= x' \sin 2\theta - y' \cos 2\theta \\ y &= x' \cos 2\theta + y' \sin 2\theta\,, \end{aligned} \quad (3)$$

the Y components of the displacements $s(\sigma)$ and $t(\sigma)$ are then equal. We obtain the following results:

$$s(\sigma) = -\sin 2\theta \sec\sigma\sqrt{(r^2 - \sin^2\sigma)} - \tan\sigma\ (1+\cos 2\theta) \quad (4)$$

$$t(\sigma) = +\sin 2\theta \sec\sigma\sqrt{(r^2 - \sin^2\sigma)} - \tan\sigma\ (1+\cos 2\theta)\,. \quad (5)$$

The width of the diffracted beam is accordingly

$$t(\sigma) - s(\sigma) = 2\sin 2\theta \sec\sigma\sqrt{(r^2 - \sin^2\sigma)}\,. \quad (6)$$

Noting that $-t(-\sigma) = s(\sigma)$ it is clear that the requisite minimum aperture for the ω-scan technique is $2|s(\sigma)_{\max}|$. To find $|s(\sigma)_{\max}|$ we differentiate $s(\sigma)$ with respect to σ and set this result equal to zero. We find $|s(\sigma)|$ to be a maximum when

$$\tan\sigma = r\cos\theta/\sqrt{((1-r^2)(1-r^2\sin^2\theta))}\,. \quad (7)$$

Accordingly, the minimum aperture for the ω scan is

$$2|s(\sigma)_{\max}| = 4r\cos\theta\sqrt{((1-r^2\sin^2\theta)/(1-r^2))}\,. \quad (8)$$

The explicit θ dependence of the minimum receiving aperture for the ω scan was not reported by Alexander & Smith (1962); moreover, we have been unable to arrive at the results given by our equations (7) and (8) following the derivation as presented in their Appendix D.

To determine the minimum aperture for the 2:1 scan it is first necessary to determine the relative displacement (as a function of σ) of the midpoint of the detector aperture and the mid-ray of the diffracted beam. The sum of this displacement and half the width of the diffracted beam is then one-half the requisite minimum aperture. When the crystal rotates through σ, the detector rotates through 2σ; the midpoint of the detector aperture is at $(-\sin 2\sigma, \cos 2\theta)$. The mid-ray of the diffracted beam intersects line IV at $\frac{1}{2}[s(\sigma)+t(\sigma)]$ and its slope is $\tan(90°+\sigma)$. The intersection of the mid-ray with the line which is the trace of the detector is at

$$(-\tan\sigma\{1+\cos 2\sigma\cos 2\theta\},\ -2\sin^2\sigma\cos 2\theta + 1).$$

The displacement between this point and the midpoint of the receiving aperture, $u(\sigma)$, is found by procedures analagous to those used above.

$$u(\sigma) = \tan\sigma\ (1-\cos 2\theta)\,. \quad (9)$$

Since the diffracted beam width is given by equation (6) we have for the aperture $v(\sigma)$,

$$v(\sigma) = 2\{\tan\sigma(1-\cos 2\theta) + \sin 2\theta\sec\sigma\sqrt{(r^2 - \sin^2\sigma)}\}\,. \quad (10)$$

To find the minimum aperture we require the value of σ which will maximize $v(\sigma)$. Differentiating $v(\sigma)$ with respect to σ we find $v(\sigma)$ to be a maximum when

$$\tan\sigma = r\sin\theta/\sqrt{((1-r^2)\ (1-r^2\cos^2\theta))}\,. \quad (11)$$

Comparing equation (11) with (7) it is interesting to note that the value of σ which maximizes the aperture for the ω scan is different from the value of σ which maximizes the aperture for the 2:1 scan. Upon substituting the value of $\sigma_{\max}$ from equation (11) into equation (10) and simplifying we find the requisite minimum aperture to be

$$v(\sigma_{\max}) = 4r\sin\theta\sqrt{((1-r^2\cos^2\theta)/(1-r^2))}\,. \quad (12)$$

This result does not agree with the result obtained by Alexander & Smith (1962) as indicated in their equation (D·9) where (taking $R_x/R_z = 1$) the θ dependence is reported as $[1-\cos 2\theta]$.

From equations (8) and (12) it is seen that the requisite minimum aperture for the ω scan is 90° out of phase with the requisite minimum aperture for the 2:1 scan. The maximum value of the minimum aperture is $4r/\sqrt{(1-r^2)}$, equivalent to twice the angle subtended by the crystal at the source, for both cases. At $\theta = 45°$ the minimum aperture for both the 2:1 and ω-scan techniques are the same.

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