It is possible to calculate such an integral by a very simple method, the application of which is limited neither by the shape of the crystal nor by its absorption power. The precision of the result can be fixed at will. The method of calculation is suitable for computer programming.

The principles of this method are as follows:

(1) Preliminary operations: the equations of the crystal faces, of the incident beam and of the diffracted beam must be given in cartesian coordinates.

(2) A point is chosen at random inside the volume of the crystal (this is why the method is a Monte Carlo one).

(3) One calculates the length of the X-ray path from the crystal surface to the point (incident beam) and from the point to the crystal surface (diffracted beam).

(4) The value of $\exp(-\mu l)$ is calculated and memorized.

(5) Another point is chosen at random, the corresponding value of $\exp(-\mu l)$ is calculated and memorized, and so on.

(6) After values of $\exp(-\mu l)$ have been obtained up to a predetermined number (100 in our program), a first average value, A_{100}, is calculated along with the r.m.s. deviation σ. Since the r.m.s. deviation $\sigma(N)$ of the average of N values is

$$\sigma(N)=\sigma/\sqrt{N}$$

one can deduce the number N of $\exp(-\mu l)$-values which must be calculated to obtain a new average with a predetermined r.m.s. deviation $\sigma(N)$. The calculations of $\exp(-\mu l)$-values are continued until N such values have been collected, and the final average is the required transmission factor.

The six steps outlined above are sufficiently clear as a general description of the method, but to make its application easier, it is well to explain steps (1), (2), and (3) in greater detail. No further explanation seem to be necessary for steps (4), (5), and (6).

In programming our calculation we use three coordinate systems one after the other: the first, whose axes are xyz, is the direct reference system, which in general is non-orthogonal; the second, whose axes are $x_0y_0z_0$, is orthogonal, where $x_0=x$, y_0 is the normal to x in the plane xy; the third, whose axes are $x_dy_dz_d$, is again orthogonal, where x_d is the projection of the incident beam on the reflexion plane, and z_d is the normal to the reflexion plane. Obviously the first two reference systems are valid for any diffraction, whereas the third varies according to the diffraction in question.

At the beginning, the first system (x,y,z) is used to obtain the coordinates of the crystal vertices, the equations of the crystal faces, the equation of the conic surface including all possible incident beams and the equation of the conic surface including all possible diffracted beams of a selected diffraction triplet. After that, all these coordinates and equations are transformed to the second (orthogonal) system $x_0y_0z_0$

The equations of the two straight lines which are the intersections of the incident-beam-cone and the diffracted-beam-cone are then deduced. The resultant coordinates and equations are then further transformed to the system $x_dy_dz_d$. A point O_1 is chosen at random inside the crystal volume. The origin of the system is set at O_1. Now the incident and the reflected beams are lying in the x_dz_d plane. The coordinates of the points along the incident beam where it meets each of the crystal faces (produced if necessary) are calculated; only the nearest point is relevant; the length of the path of the incident beam is calculated; the same is done for the diffracted beam. The value of $\exp(-\mu l)$ is now readily calculated. The calculation continues as indicated in steps (4), (5), and (6).

On this basis a FORTRAN program has been compiled, which is suitable for crystals of any absorption and form (provided they have no re-entrant angles) and for intensities measured from Weissenberg and Buerger photographs. On an IBM 7094 computer the time needed for assemblage is about two minutes, the time needed to calculate one transmission factor for a crystal of rather simple form (6 faces, maximum length 0·2 mm) with a r.m.s. error of 3% is about 14 seconds. The computing time is proportional to the square of the precision required, to the number of the crystal faces and to μ times the dimensions of the crystal. The program can easily be adapted for use with other experimental data, or with crystals with re-entrant angles, or with curved boundaries.

Our method of calculating transmission factors has some features similar to the method of Busing & Levy (1957). Recently Coppens, Leiserowitz & Rabinovich (1965) and, a few months later, Wuensch & Prewitt (1965) have redescribed the Busing & Levy (BL) method, in a way suitable for general application. The BL method differs from ours mainly in that the X-ray path is calculated for a regularly spaced grid of points. The precision obtained is known only at the end of the calculation, and, if greater precision is needed, the calculation must be done again. With our method the precision is predetermined at will.

As far as the difficulty of programming is concerned, our method is very simple. The BL method with its Gaussian quadrature seems to be more complicated from this point of view. The computing time of the BL method could be shorter, but we are unable to predict this with certainty, as until now a general program of the BL method is not available to us. In any case our program is not very time-consuming.

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The α_1, α_2 splitting correction for non-integrated Weissenberg X-ray intensity photographs.

By E. G. BOONSTRA, *National Physical Research Laboratory, Council for Scientific and Industrial Research, P.O. Box* 395, *Pretoria, South Africa*

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The diffraction spots recorded with a non-integrated Weissenberg camera are generally split owing to the α_1, α_2 doublet of the characteristic $K\alpha$ X-ray line. Rae & Barker (1961) studied microphotometer traces of such spots and have derived a correction factor $C(\theta)$ which is applied to the measured peak height to yield the integrated intensity

for each spot. It is clear from their formulation that the spot separation is given as $\Delta(2\theta)$, and this can only be the case for a normal-beam zero-level photograph where the film coordinate Y equals 2θ directly. In fact, the numerical examples used to illustrate the correctness of their expression are for $hk0$ intensities. It is the purpose of this note to examine the validity of their result for other camera settings which are used to collect three-dimensional intensity data. The symbols used in this treatment are the standard ones originally defined by Buerger (1962) and those introduced by Rae & Barker.

Assume that the intensity ratio of the spots due to the α_1, α_2 doublet is $r(\geq 1)$, that the intensity distribution for each is triangular with halfwidth b and that their separation is $\Delta(Y)$, both in angular measure. The correction factor C is applied to the resultant peak height when the spots are not resolved ($\Delta \leq b$) or to the maximum peak height when the spots are partially resolved ($b \leq \Delta \leq 2b$) or completely resolved ($\Delta \geq 2b$). Then it can be shown that

$$C = 1 + 1/[(1+r)b/\Delta - 1] \text{ for } \Delta \leq b$$
$$C = 1 + 1/r \qquad \text{for } \Delta \geq b$$

The problem then is to express Δ in terms of the parameters of the spot position, diffraction conditions and camera settings. For the general case where a reciprocal lattice level is recorded with inclination angle μ of the camera and level setting ν of the screen, it may be shown that the film coordinate Y of a reflexion is given by

$$\cos Y = (\cos 2\theta - \sin \nu \sin \mu) \cos \mu \cos \nu .$$

The spot separation can then be expressed as

$$\Delta = \Delta(Y) = (dY/d\lambda)\Delta\lambda$$
$$= \operatorname{cosec} Y d(\cos Y)/d\lambda \Delta\lambda$$

where

$$d\mu/d\lambda = 0$$
$$d\nu/d\lambda = (\sin \nu - \sin \mu)/\lambda \cos \nu$$
$$d\theta/d\lambda = \tan \theta/\lambda ,$$

and after differentiation and substitution one obtains the result

$$\Delta(Y) = (\Delta\lambda/\lambda) \frac{[\cos \nu(1 + \cos^2\mu - \sin \nu \sin \mu) - \cos \mu \cos Y (1 + \cos^2\nu - \sin \nu \sin \mu)]}{\sin Y \cos \mu \cos^2\nu} .$$

The straight-through position on the film is given by $Y = 0$, and one would normally expect the splitting to vanish there. This is true only for $\mu = \pm\nu$, *i.e.* equi-inclination or anti-equi-inclination setting which includes the normal-beam zero-level case discussed by Rae & Barker. We find for these three cases the following results:

(i) Normal-beam zero-level $\mu = 0$, $\nu = 0$ and $Y \equiv 2\theta$

$$\Delta(Y) = 2(\Delta\lambda/\lambda) \tan Y/2 = (2\Delta\lambda/\lambda) \tan \theta$$

in agreement with Rae & Barker.

(ii) Equi-inclination $\mu = -\nu$

$$\Delta(Y) = (2\Delta\lambda/\lambda) \tan Y/2/\cos^2\nu .$$

(iii) Anti-equi-inclination $\mu = \nu$

$$\Delta(Y) = (2\Delta\lambda/\lambda) \tan Y/2 .$$

For any other case, such as a normal-beam upper-level photograph where $\mu = 0$ the result is more complicated and one can expect the splitting to vanish at some value of Y, below which the splitting would be anomalous. If such a method of recording intensity photographs is used, the general expression given above will have to be evaluated for that particular case.

The half-width of the unresolved spot is still given by $\sigma = b + \Delta/1 + r)$, and it follows that, for the three special cases considered, the value of b can be obtained by plotting the measured half-width σ for low Y values against $\tan Y/2$ and extrapolating to zero Y. In the equi-inclination case the slope will differ by a factor $\cos^2\nu$ from the anti-equi-inclination case. After the value for b has been obtained the factor $C(Y)$ can be tabulated along the lines suggested by Rae & Barker.

There is another convenient way in which the correction factor can be formulated. Let Y_0 be the value of Y above which the spots are completely resolved. Then

$$C = 1 + 1/r \qquad \text{for } Y \geq Y_0$$
$$= 1 + 1/[(1+r)d_0/d - 1] \text{ for } Y \leq Y_0 ,$$

where

$$d = \tan Y/2$$

and

$$d_0 = \tan Y_0/2 \text{ (for the three special cases)} .$$

It is suggested that this method of applying the correction factor may be simpler than that employed by Rae & Barker. Instead of the parameters λ, $\Delta\lambda$ and b (deduced by extrapolation), only the one parameter Y_0 (obtained directly from the film) is used.

The method of Rae & Barker has been rigorously extended to cover with minor alterations the case of equi-inclination and anti-equi-inclination settings, which includes normal-beam zero-level photographs. For the general case, more complicated expressions are required, and this includes the case of normal-beam upper-level photographs, where the splitting will be anomalous near the centre of the film.

Although these results may not affect the actual value of the correction factor greatly, it is satisfying from a computational point of view to use the correct analytical expression for the factor. The factor as derived is applied to photometrically measured peak heights, but since visual intensity measurements are generally believed to estimate maximum photographic density, it follows that this factor can be applied to both visually and photometrically measured intensities.

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