and therefore increases as the scale of the apparatus is increased.

6·4·2. *Effect of fixed specimen size.*—Consider first the dimensions arranged so that the value a at which the specimen size is fixed is the optimum value for the particular focal distance (s) being used, the focal size (f) being also given its optimum value. Then, as in (18),

$$s = 6la,\ f = 3a,\ d = s/2\ .$$

Now, if a smaller value of s were used, and if a and f were adjusted to their optimum values (for this new value of s), then, by (19), the resultant intensity at the film would *decrease*. Therefore, the optimum value of s for a given value of a must be in the region where $s \geqslant 6la$. Consider now values of s in this range.

If the intensity expression (4) (with I_0 now made $\propto 1/f^{\frac{1}{2}}$) is differentiated with regard to f, the optimum value of f for a given value of a and s is seen to be

$$f = \frac{6s+la-\sqrt{(l^2a^2+48las)}}{2l}. \qquad (20)$$

If the overlap condition is to be obeyed, then by substituting $f \leqslant s/2l$ in (20) one readily obtains

$$s \leqslant \frac{38la}{25}.$$

Therefore, the optimum value of focal size given by (20) cannot be reached in the region where $s \geqslant 6la$.

Inspection of (4) shows that the intensity at the film increases from zero when $f = 0$, and would in theory reach a maximum at the value of f given by (20); thus the best value of f is the maximum permissible for overlap, i.e.

$$f = s/2l\ .$$

The intensity expression now reduces to

$$I \propto \frac{(s-2la)^2}{s^{5/2}}. \qquad (21)$$

Differentiating this expression with regard to s, the maximum value of intensity is found to occur when

$$s = 10la,\ f = 5a,\ d = 5la\ . \qquad (22)$$

6·4·3. *Focal size fixed.*—In this case, as the power loading will be constant, the optimum conditions must be the same as for the stationary-anode fixed-focus case. That is,

$$a = f/3,\ s = 2lf,\ d = lf\ ,$$

as in equation (13).

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A Method for the Estimation of Transmission Factors* in Crystals of Uniform Cross Section

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This article presents a method of estimating the transmission factors of crystals with uniform cross section. It synthesizes Albrecht's idea of dividing the section into parallelograms and measuring the path length x for the centre of each, with Howells's loci of points of constant x. Thus, bands of approximately constant x are obtained, which make the computations very quick. An example and a detailed discussion on the accuracy to be expected are also given.

1. Introduction

While working on the determination of the crystal structure of the strongly absorbing sodium–thyroxine ($\mu = 437$ cm.$^{-1}$) the intensities of the diffracted beams had to be corrected for absorption.

The best method known to us for estimating the transmission factors was that of Howells (1950) by which these factors can be calculated very conveniently with any degree of accuracy required. Although it is very quick for some particular advantageous cases, it may become involved in some others, requiring a

* The authors think that the name of transmission factor is more appropriate than the generally accepted name of absorption factor, as it actually gives the fraction of radiation transmitted by the crystal.

calculation which includes all the parts of the graph explained in that article.

To obtain quicker, though less accurate, results, the method published by Albrecht (1939) was tried. He divided the section of the crystal into parallelograms with sides parallel to the directions of the incident and diffracted beams, measured the path length, x, travelled in the crystal by the rays diffracted from the center of each parallelogram, and calculated

$$T_{hk0} = (1/n) \Sigma \exp [-\mu x] ,$$

where T_{hk0} is the ratio I'_{hk0}/I_{hk0} between the observed intensity and the ideal intensity had no absorption occurred.

This method did not prove to be very helpful, as rather a great number of path lengths had to be measured, and many fractions of parallelograms had to be computed as well.

2. The new method

It occurred to one of us (R.V.) that Albrecht's idea would lead to an extremely simple method if use was made of Howells's loci of points with constant x. Instead of dividing the section of the crystal in directions parallel to the incident and diffracted beams, it is first divided (as in Howells's method) into regions so that each region contains all the points which diffract beams entering and leaving the crystal through two given faces (these two faces may of course be the same one); then each one of these regions is in turn divided, by means of lines parallel to the locus of points with constant x (Fig. 1), into bands whose width is constant within each region.

In his paper, Howells gives a rule for determining both analytically and geometrically the loci in the example given there. A general rule is the following: At any point P draw two straight lines PA and PB of equal length parallel to the incident and diffracted beams respectively, both being either in the direction of the X-rays or in the opposite direction. Through A draw a line parallel to the entrance face, and through B a line parallel to the exit face. If these two lines meet at M, the locus in that region is parallel to PM. Of course, it is much more convenient to choose P at the intersection of the lines dividing the section of the crystal into regions if these lines intersect inside the drawing—or at least on one of them if they do not—and to choose A or B at one of the vertices. This will save lines and make the operation quicker and more accurate. It is obvious that if the entrance face and the exit face are parallel, the locus will be parallel to them too.

Having drawn the parallel lines in one region—preferably the simplest one—the system of parallel lines in the neighbouring region is drawn through the points at which the lines of the first region intersect the border line between the two (Fig. 1). In this way, the bands may extend throughout more than one region. The path length x for all the points of one such polygonal is obviously constant, and therefore will be approximately the same for all points within such a complete band.

The determination of the transmission factor requires now only a scale drawing of the crystal section, divided into the corresponding regions by the directions of incidence and diffraction, the determination of the directions of the loci, the drawing of the systems of parallel lines, the estimation of the areas s of each complete band (see Fig. 1), the determination of the corresponding values of x—taken at points equidistant from the two edges of the band—and the calculation of

$$T_{hk0} = \Sigma s \exp [-\mu x]/\Sigma s ,$$

where s is the area of the complete band for which the path length is approximately x.

The values of s may be determined either directly or, for greater accuracy, as follows: If the region is a parallelogram with one pair of sides parallel to the bands, s is constant throughout it and is easily estimated. If the region, or part of it, is a triangle with one side coincident with an edge between bands, the increment Δs between one band and the next is $2A/n^2$, where A is the area of the triangle and n (preferably integral) is the number of bands in it. The values of s are then, starting from the vertex: $\frac{1}{2}\Delta s$, $\frac{3}{2}\Delta s$, $\ldots \frac{1}{2}(2n-1)\Delta s$. If the region does not be-

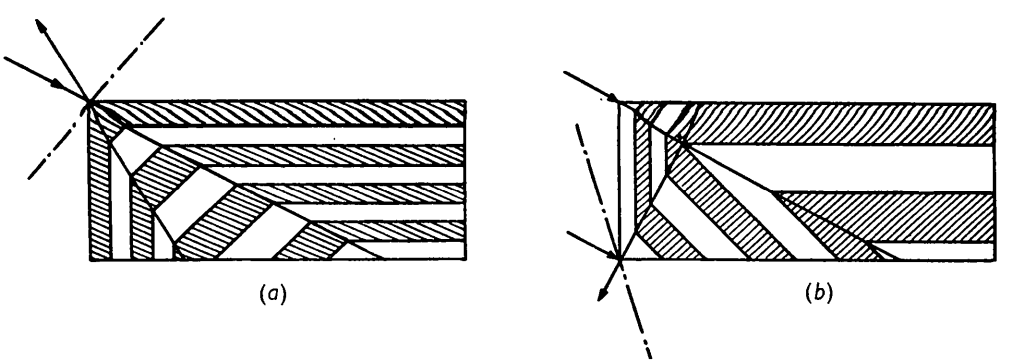

Fig. 1. Two examples showing how the crystal section is divided into bands of approximately constant x, and how the bands may extend throughout more than one region.

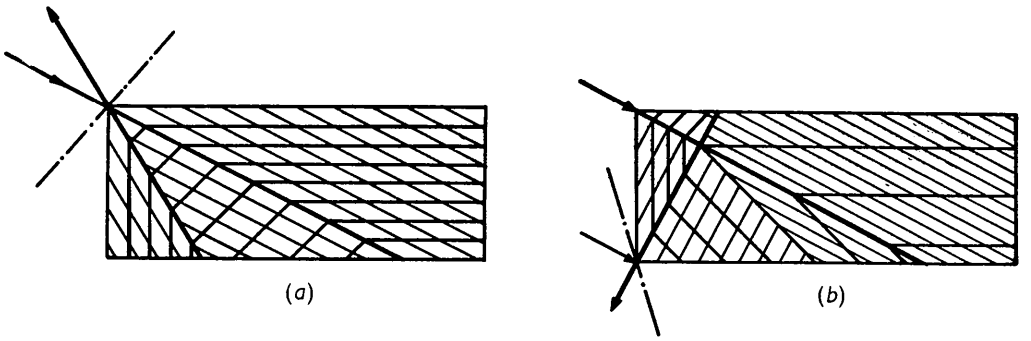

Fig. 2. The examples of Fig. 1, in which the bands have been divided into parallelograms of equal area.

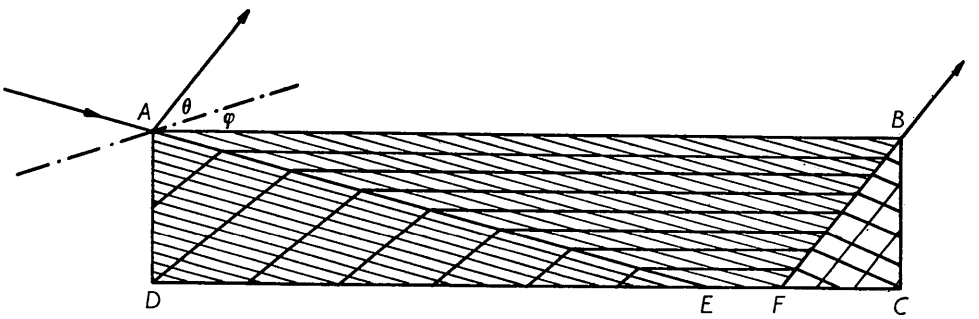

Fig. 3. Illustration of the example worked out in detail in § 3.

long to any of the above-mentioned cases, it may be always divided into parallelograms and triangles which do belong to them.

The accuracy in the estimation of the values of s may be checked since Σs must be equal to the area of the crystal section.

As x varies linearly throughout one given region, the increment in μx between adjacent bands is given by $\mu\Delta x = \mu(X_2 - X_1)/n$, where X_2 and X_1 are respectively the longest and the shortest path lengths in the region (X_1 is very often zero) and n is the number of bands in the region. As the path lengths x are computed for points in the middle of each band, the first value of μx is obtained by adding to μX_1 the value of $\frac{1}{2}\mu\Delta x$. Values for the remaining bands are obtained by successive additions of $\mu\Delta x$.

Another procedure is to divide each region again by another set of parallel equidistant lines, to form parallelograms (and fractions of parallelograms). The new direction is that of the incoming rays, that of the outcoming rays, or that of the locus of a neighbouring region, and the parallelograms are built up in such a way as to obtain the least number of fractions. This may require a change in the direction of the second set of parallel lines even within one region. Now, instead of measuring the areas of each complete band, the number of parallelograms in it is counted. Of course, this requires all the parallelograms to have the same area, and this is easily achieved (Fig. 2).

In some cases it is not necessary to draw all the parallelograms, but only the fractions close to the border line; the number of whole parallelograms is easily calculated from the scale drawing.

The transmission factor becomes:

$$T_{hk0} = \Sigma p \exp[-\mu x]/\Sigma p ,$$

where p is the number of parallelograms in the band for which the path length is approximately x (p is not necessarily integral).

Similar considerations to those given above for the determination of s apply here for the determination of p; and the values of μx are calculated in exactly the same way.

For a given crystal, the accuracy in the result depends on the accuracy of the drawing and of the estimation of the fractions of parallelograms, and on the width of the bands. The extent to which the width of the bands may influence the result may be seen in the following examples. In these examples the range of x that has to be considered will also be discussed because very long path lengths contribute very little to the transmission factor.

3. Example

The cross-section $ABCD$ of the crystal is rectangular, $0{\cdot}020 \times 0{\cdot}004$ cm. (Fig. 3). The reflecting plane forms with AB an angle $\varphi = 18°$ and its Bragg angle is $\theta = 33°$. Thus, the incident beam forms with AB an angle $\varphi - \theta = -15°$, and the diffracted beam forms with AB an angle $\varphi + \theta = 51°$. (The values of φ and θ

for any plane may be easily obtained from the reciprocal lattice). Let μ be 400 cm.$^{-1}$.

The central region, in which the loci are parallel to AB, is divided into 8 bands. Then the bands in the other two regions are drawn, parallel to the corresponding loci, and they are divided into parallelograms, as explained in § 2.

$X_1 = 0$, $X_2 = AE+FB = 0{\cdot}0208$ cm., $n = 8$. Thus $\mu\Delta x = \mu(X_2-X_1)/n = 1{\cdot}04$ and $\frac{1}{2}\mu\Delta x = 0{\cdot}52$.

Data for all the bands are given in Table 1.

Table 1

Band	μx	exp $[-\mu x]$	p	p exp $[-\mu x]$
1	0·52	0·595	22·9	13·63
2	1·56	0·210	28·6	6·01
3	2·60	0·074	29·4	2·18
4	3·64	0·026	25·1	0·65
5	4·68	0·009	20·9	0·19
6	5·72	0·003	16·7	0·05
7	6·76	0·001	11·3	0·01
8	7·80	$0{\cdot}000_4$	4·8	$0{\cdot}00_2$
			159·7	22·72

$T = 22{\cdot}72/160 = 0{\cdot}142$.

4. Discussion of the accuracy of the method

To show how the accuracy of the result depends on the subdivision, the values of T_n (for $n = 4$, 8, 16) and T_H (calculated with Howells's method) are given below for the same diffraction plane as in the preceding example. T_H is the exact value, and the percentages of error are referred to it.

$T_4 = 0{\cdot}130$	12% error
$T_8 = 0{\cdot}142$	3% error
$T_{16} = 0{\cdot}145$	1% error
$T_H = 0{\cdot}147$	0% error

Table 2

μ	100	200	400	800	1600
T_4	0·485	0·284	0·130	0·041	0·005
T_8	0·489	0·289	0·142	0·060	0·018
T_{16}	0·491	0·290	0·145	0·066	0·027
T_H	0·493	0·292	0·147	0·068	0·032

Table 3

$\mu\Delta x$	μ	n	%
0·26	100	8	0·8
	200	16	0·7
0·52	100	4	1·6
	200	8	1·0
	400	16	1·4
1·04	200	4	2·7
	400	8	3·4
	800	16	2·9
2·08	400	4	11·6
	800	8	11·8

The combined effect of μ and Δx is shown in Table 2 for the same diffraction plane.

Table 3 gives the percentages of error in T_n as compared with T_H, in groups of constant $\mu\Delta x$ (or constant μ/n). This table shows that the error is approximately constant for a given value of $\mu\Delta x$, and increases rapidly with it. Although these errors may vary for different diffraction planes and for different crystal sections, they give an idea of the value of $\mu\Delta x$ to be chosen in order to obtain a given accuracy.

5. The effect of neglecting large values of μx

The extent to which large values of μx may be neglected is shown in Table 4, in which T_{8i} represents the value of T_8 calculated from Table 1 by adding only the i first terms ($i = 1, 2, \ldots, 8$). The next column shows the percentages of error, referred to T_{88} (which is obviously equal to T_8). The last column shows the highest value of μx computed in each case.

Table 4

i	Σp exp $[-\mu x]$	T_{8i}	%	μx
1	13·63	0·085	40	0·52
2	19·64	0·123	13	1·56
3	21·82	0·136	4·2	2·60
4	22·47	0·140	1·4	3·64
5	22·66	$0{\cdot}141_6$	0·3	4·68
6	22·71	$0{\cdot}141_9$	0·1	5·72
7	22·72	$0{\cdot}142_0$	0·0	6·76
8	$22{\cdot}72_2$	$0{\cdot}142_0$	0·0	7·80

Table 4 shows—unless p increases too rapidly with μx—the highest value of μx that need be computed in the calculation of the transmission factor. It can be shown that for sufficiently narrow bands, and if p (or s) has the same value for all the bands, the ranges of μx to obtain errors of 10%, 1%, 0·1%, etc. are: 2·3 ($= \log_e 10$), 4·6, 6·9, etc. If the bands are too wide (small n) and the value of p increases rapidly with μx, the corresponding ranges of μx to be computed are greater.

It is most important to remember that, even when some bands are neglected because of their high μx values, Σs and Σp mean the area of the complete crystal section, including the neglected areas.

As a final remark, it may be noticed that if μ is small, n may be small too (wide bands); and that if μ is large, also n has to be taken large (narrow bands), but in this case only a few bands need be computed as the large values of μx are neglected.

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