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The Formula for Integrated Intensity from Extended-Face Imperfect Crystals – Inclusion of Surface-Layer Effects

By A. McL. Mathieson

Division of Chemical Physics, CSIRO, P. O. Box 160, *Clayton, Victoria, Australia* 3168

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By reference to intensity measurements made with an asymmetrically cut extended-face lithium fluoride crystal, attention is drawn to (*a*) the observation that the average of measurements at asymmetrical angles $+\alpha$ and $-\alpha$ is not always equal to the value at the symmetrical position, $\alpha=0°$, as implied by W. H. Bragg [*Phil. Mag.* (1914), **27**, 881–899] and accepted as essentially correct by later experimentalists; and (*b*) the associated consequence that the conclusions of Hirsch and his colleagues concerning extended-face crystals arrived at *ca.* 1950 [*e.g.* Gay & Hirsch, *Brit. J. Appl. Phys.* (1951). **2**, 218–222] are of general rather than specific significance. It is deduced that the standard formula for the absorption factor, A_c, for such crystals [*International Tables for X-ray Crystallography* (1967). Vol. II], should be modified to incorporate an additional component of the form

$$\exp\{-\mu't[\operatorname{cosec}(\theta+\alpha)+\operatorname{cosec}(\theta-\alpha)]\},$$

where μ' is the effective absorption factor for the surface layer of thickness t and α is the angle between the surface and the Bragg plane studied. The formula for the integrated intensity is then given by

$$\frac{E\omega}{I}=\frac{Q}{2\mu}(1-\cot\theta\,.\,\tan\alpha)\,.\,\exp\{-\mu't[\operatorname{cosec}(\theta+\alpha)+\operatorname{cosec}(\theta-\alpha)]\},$$

which reduces in the symmetrical case, $\alpha=0°$, to

$$\frac{E\omega}{I}=\frac{Q}{2\mu}\,.\,\exp(-2\mu't\operatorname{cosec}\theta)\,.$$

The factor $\mu't$ can be determined experimentally by use of an appropriately prepared asymmetrically cut crystal or by selection of a reflexion plane at an angle to the surface used for measurement. The onus should be on the experimenter to establish the magnitude of the factor and hence whether its incorporation is mandatory. Its omission in application of this technique for the determination of structure factors may have significant effects on scale factors, particularly where absolute values are sought, and on derived temperature factors and extinction parameters.

Introduction

Most of the early quantitative measurements of X-ray intensities were made with extended-face crystals. Because of the current concern with increased accuracy in the determination of structure factors [see, for example, IUCr (1969)] this technique is receiving renewed attention (Barnea, 1975).

In a classical paper, W. H. Bragg (1914) noted that when the crystal face was at an angle α to the reflexion plane studied (Fig. 1), the measured value of integrated intensity differed from that at the symmetrical position when $\alpha=0°$. This observation was of practical importance since extended-face crystals generally have prepared surfaces and it is not always possible for these to be exactly parallel to the relevant crystal plane. To eliminate this effect, Bragg advocated measurement with the incident beam first at $\theta+\alpha$ [Fig. (1*a*)] and then at $\theta-\alpha$ [Fig. 1(*c*)] to the crystal face, the two readings being averaged to yield a value of integrated intensity which he assumed as equivalent to the value in the symmetrical position.

There appears to have been no investigation of the general need for any further essential experimental correction to be applied using the procedure on imperfect ('mosaic') crystals – see for example, *International Tables for X-ray Crystallography*, (1967); Mair, Prager & Barnea (1971); Lawrence (1972).

In the process of investigating asymmetric reflexion from an extended-face crystal in relation to work on a 'defocusing' monochromator (Mathieson, 1975), it became evident that, for such crystals in general, under symmetrical as well as asymmetrical conditions, recognition of the existence of a further correction is necessary, one which is particularly relevant for crystals with a prepared (abraded) surface. The magnitude of the correction can be assessed experimentally.

Since the correction is dependent on θ as well as on the thickness of the surface layer, its recognition is not merely of theoretical concern but has relevance to the practical procedures of measurements in the establishment of structure factors of improved accuracy, particularly in placing experimental data on an absolute scale.

Background

Evans, Hirsch and Kellar in Cambridge, England, initiated studies of asymmetric reflexion with extended-face crystals, which spanned the period 1948–1952. Motivad by an investigation on a 'concentrating' monochromator (Evans, Hirsch & Kellar, 1948), the studies paid particular attention to matters of *specific intensity*. Experimentally, the region of positive α, Fig. 1(*a*), usually from $\alpha=0^\circ$ to $\alpha=+\theta^\circ$, was explored. The results for a number of different crystals could be interpreted in terms of the existence of an absorbing but non-reflecting surface layer which was produced by the abrading or polishing technique used in preparing the samples. The experimental approach was diversified providing a non-destructive method for the determination of the thickness of surface layers (Gay & Hirsch, 1951) and also placing outer bounds on the value of structure factors, exemplified for two reflexion orders from two samples of natural quartz (Gay, 1952). This latter study utilized the theoretical work of Hirsch & Ramachandran (1950) on asymmetric reflexion from perfect and imperfect crystals.

In the work of the Cambridge group, the concentration on *specific intensity* with the consequent need to account for exact details of beam breadth for incident and diffracted beams, the latter of which changes with α, led to formulae which, while well suited to the purpose of the authors, apparently caused the more general significance of these studies to be overlooked. In fact, the general conclusions reached in the present paper are implicit in the work of the Cambridge group but their functional relevance has not been explicitly recognized in the intervening 20+ years, to judge from standard reference sources (James, 1948; *International Tables for X-ray Crystallography*, 1967) and from experimentalists in the field (Mair, Prager & Barnea, 1971; Lawrence, 1972).

Observations

For the purpose of our experiment, a near-cylindrical boule of lithium fluoride of about 2.5 cm diameter and 1.2 cm height was used, the base being parallel to (200) and the top surface being ground at 15° to the base. The experimental procedure to allow variation of α was the same as in Evans, Hirsch & Kellar (1948). The crystal was mounted on a Picker diffractometer and adjusted so that the pole of (200) coincided with the ϕ axis of the instrument. Because of the changing breadth of the diffracted beam with change of α, all apertures normally present between the specimen and the sensitive surface of the scintillation detector were removed.

Measurements on 200 ($\theta \simeq 22{\cdot}5^\circ$ for Cu $K\bar{\alpha}$) were carried out at 10° intervals in ϕ (Fig. 2). A polar diagram of the results is shown in Fig. 3. Symmetry about the line $\phi=90^\circ$ to 270° is evident. The variable ϕ can be converted to the variable α by the relationship, $\tan\alpha=\sin\phi\tan\alpha_0$ (Evans, Hirsch & Kellar, 1948), α_0 being the maximum slope of the ground surface relative to (200).

It can be seen that the mean of values at $+\alpha$ and $-\alpha$ is not exactly equal to the value at the symmetrical position, $\alpha=0^\circ$, as Bragg (1914) had implied and as is deduced in James (1948). Fig. 4 illustrates the trend with $|\alpha|$.

It is of interest to look more closely at the experimental data. The viewpoint adopted here differs slightly from that of the Cambridge group in respect of the physical situation. Our concern is with *total*, *i.e.* integrated, intensity rather than with *specific* intensity. Also we deal here with the region $-\alpha$ as well as $+\alpha$,

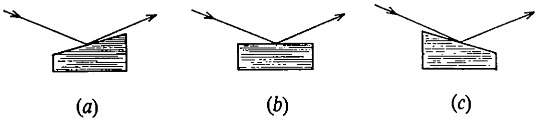

Fig. 1. Reflexion from an extended-face crystal: (*a*) asymmetrical with $+\alpha$, (*b*) symmetrical with $\alpha=0^\circ$, (*c*) asymmetrical with $-\alpha$. Incident beam is from the left in each case.

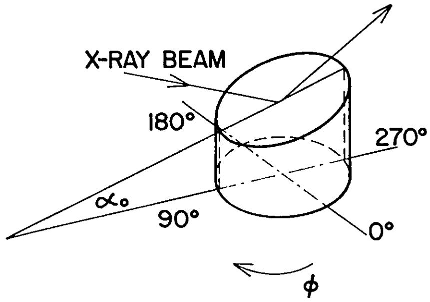

Fig. 2. Crystal with an asymmetrical surface at α_0 to the base, which is parallel to the reflexion studied, 200. The pole of (200) and the rotation axis ϕ coincide.

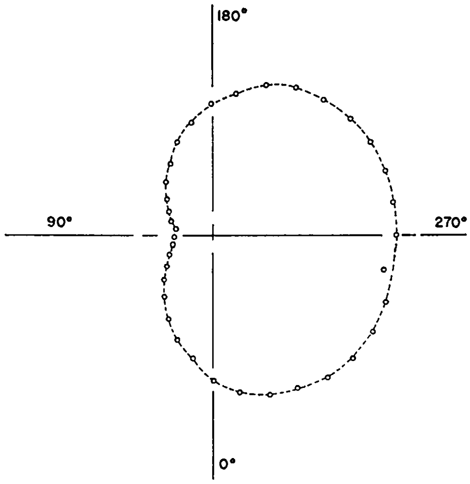

Fig. 3. Polar diagram of integrated intensity $I(\phi)$, measured when the incident beam is in the plane defined by the ϕ axis and the specified value of the angle ϕ.

whereas the Cambridge group dealt wholly with the latter region (see Fig. 1).

If we consider the relationship for the integrated intensity from an extended-face crystal whose surface is at an angle $+\alpha$ with respect to the reflexion plane studied, this, according to James (1948), is given by

$$\frac{E\omega}{I}=\frac{Q}{2\mu}\cdot(1-\cot\theta\cdot\tan\alpha)\,. \qquad (1)^*$$

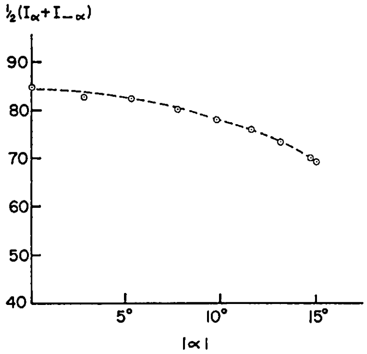

Fig. 4. Variation of the mean value of $I_\alpha+I_{-\alpha}$ with $|\alpha|$.

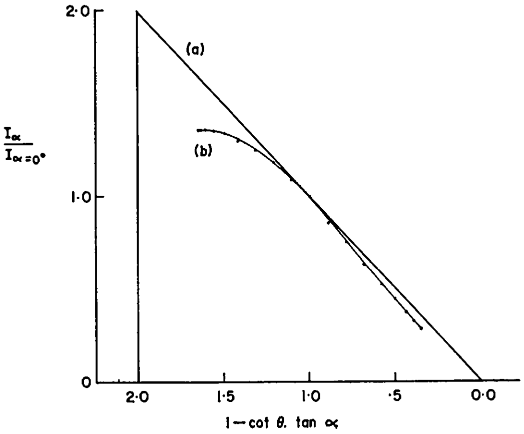

Fig. 5. Plot of intensity against $(1-\cot\theta\,.\,\tan\alpha)$: (*a*) theoretical, based on equation (1), and (*b*) experimental data, arbitrarily scaled to approximate coincidence at $\alpha=0°$.

In the symmetrical position, with $\alpha=0°$, (1) reduces to

$$\frac{E\omega}{I}=\frac{Q}{2\mu}\,. \qquad (1a)$$

The symbols used have the usual significance (*vide* James, 1948).

For variation of α over the range $+\theta$ to $-\theta$, the relationship (1) is depicted in Fig. 5(*a*). As in Fig. 4, the experimental curve, Fig. 5(*b*), deviates from the theoretical, the deviation increasing with increase in $|\alpha|$. The underlying situation is more readily revealed if one normalizes the measurements to effective equal scattering volume by

$$\frac{E\omega}{I}\left(\frac{1}{1-\cot\theta\tan\alpha}\right)=\frac{Q}{2\mu}\,. \qquad (2)$$

This is shown in Fig. 6. Here also, the experimental data drop with deviation of α from $\alpha=0°$. However, the point of note is that the experimental plot is approximately symmetrical about $\alpha=0°$. The deviation is therefore dependent on a functional variable which is symmetrical about $\alpha=0°$ – or, in other words, incident and diffracted beam paths are interchangeable. In fact, for a layer of thickness t normal to the surface, the sum of the resultant additional incident and diffracted beam paths, $t\,[\operatorname{cosec}(\theta+\alpha)+\operatorname{cosec}(\theta-\alpha)]$, is such a function. A plot of

$$\log\left(\frac{E\omega}{I}\left(\frac{1}{1-\cot\theta\tan\alpha}\right)\right)$$

versus $[\operatorname{cosec}(\theta+\alpha)+\operatorname{cosec}(\theta-\alpha)]$

(*cf.* Gay & Hirsch, 1951) yields a straight line (Fig. 7) and hence confirms the applicability of the surface-layer model of Hirsch *et al.* in respect of this specimen of lithium fluoride. It also confirms its appropriateness in the present context for spanning both positive and negative regions of α, provided the data are normalized to equal scattering volume†.

The present observations on integrated intensity in both positive and negative regions of α confirm the essential generality of the earlier observations based on specific intensity in the positive region of α. Hence the interpretation by Hirsch and his colleagues of their observations on the basis of a layer of thickness, t, of absorbing but non-reflecting material on the surface of an abraded crystal may, to a first approximation, be considered as applicable, in respect of the measurement of integrated intensity, to the present sample of lithium fluoride and indeed to any extended-face crystal whose surface has been prepared by abrasion or polishing. That it may also be applicable to natural faces with protuberances has been adumbrated by Gay (1952).

From the evidence presented here and implied in the work of the Cambridge group, it would appear essen-

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* In *International Tables for X-ray Crystallography* (1967), the formula for reflexion from crystal planes inclined at angle ϕ to the extended face of a crystal block of negligible transmission is given as

$$A_c=\frac{1}{\mu}\cdot\frac{1}{1+\dfrac{\sin(\theta+\phi)}{\sin(\theta-\phi)}}\,,$$

which reduces to

$$A_c=\frac{1}{\mu}\left(\frac{1-\cot\theta\tan\phi}{2}\right).$$

To avoid confusion with the symbol ϕ for the diffractometer axis, the symbol for the inclination angle in the text is taken instead as α.

† Certain indications of very minor distinctions between incident and diffracted beams warrant comment in another place but these are not relevant to our present observations.

tial that the general formula for the absorption factor, A_c, for an extended-face crystal should be altered to

$$A_c = \frac{1}{2\mu}(1 - \cot\theta \cdot \tan\alpha) \times \exp\{-\mu' t[\operatorname{cosec}(\theta+\alpha) + \operatorname{cosec}(\theta-\alpha)]\}\,, \quad (3)$$

which for the symmetrical case reduces to

$$A_c = \frac{1}{2\mu} \cdot \exp(-2\mu' t \operatorname{cosec}\theta)\,. \quad (3a)$$

It is not necessary that μ' be identical with μ (Gay, Hirsch & Kellar, 1952) or that t be determined. All that is necessary is that the product $\mu' t$ be established over a range of α.

It will be noted that, even in the symmetrical position, $\alpha = 0°$, as in equation (3*a*), the exponent can differ significantly from unity. Indeed, for the present case, extrapolation to zero additional absorbing path, *i.e.* $[\operatorname{cosec}(\theta+\alpha) + \operatorname{cosec}(\theta-\alpha)] = 0$ (Fig. 7) indicates that the true value of integrated intensity in the symmetrical position, with no absorbing surface layer, would be ~27% above that actually measured. In fact, correction of the experimental data by the full expression $(1 - \cot\theta \cdot \tan\alpha)^{-1} \cdot \exp\{\mu' t[\operatorname{cosec}(\theta+\alpha) + \operatorname{cosec}(\theta-\alpha)]\}$ with $\mu' t = 0{\cdot}046$ yields corrected integrated intensities (19 values) which show a mean deviation of 0·9% (Table 1).* Fig. 8(*a*) shows the distribution of these values, scaled to unity, while curve (*b*) presents the original data on the same scale, but with the surface-layer absorption correction omitted. It is evident that the curves (*b*) in both Figs. 5 and 6 should, for a correct representation relative to their respective (*a*) curves, be scaled down by a factor of ~0·8 (see Table 1). In this experiment, which has been carried out to demonstrate the existence and significance of the surface-layer absorption in relation to the measurement of integrated intensity, no special attempt was made to achieve high precison. It is clear that, in respect of the measurement of a single reflexion, failure to recognize the influence of the surface layer (or equivalent protuberances) and to establish its magnitude could lead to a serious error in scale – a matter of considerable concern since the extended-face crystal is potentially capable of yielding absolute data.

It is also evident from equation (3*a*), that, for a series of reflexions measured in the symmetrical mode, the additional absorption factor is θ-dependent, as well as $\mu' t$-dependent. Values of structure factors derived from experimental data by use of equation (1*a*) rather than equation (3*a*) will be in error, but the existence of this error is likely to be mainly obscured by compensatory errors in the temperature (*B*) factors and the extinction parameters deduced. The trend of the additional surface-layer absorption factor over the range $\theta = 5°$ to 90° for typical values of $\mu' t$ (0·05, 0·015,

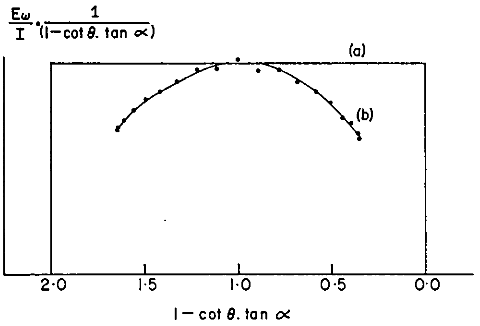

Fig. 6. Plot of $(E\omega/I)$ $(1 - \cot\theta\,.\,\tan\alpha)$ against $(1 - \cot\theta\,.\,\tan\alpha)$; (*a*) theoretical, based on equation (2); (*b*) experimental data, arbitrarily scaled to approximate coincidence at $\alpha = 0°$.

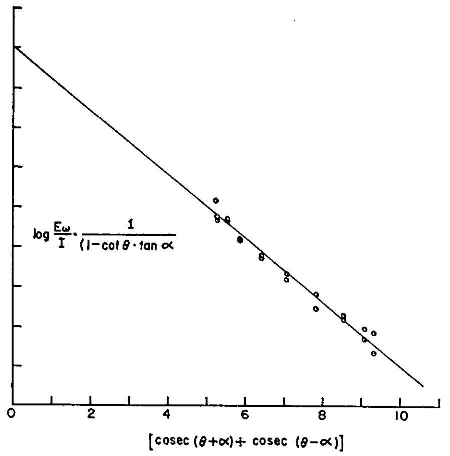

Fig. 7. Plot of $\log[(E\omega/I)\,(1 - \cot\theta\,.\,\tan\alpha)^{-1}]$ against $\operatorname{cosec}(\theta+\alpha) + \operatorname{cosec}(\theta-\alpha)$. From the slope a value of $\mu' t = 0{\cdot}046$ is derived.

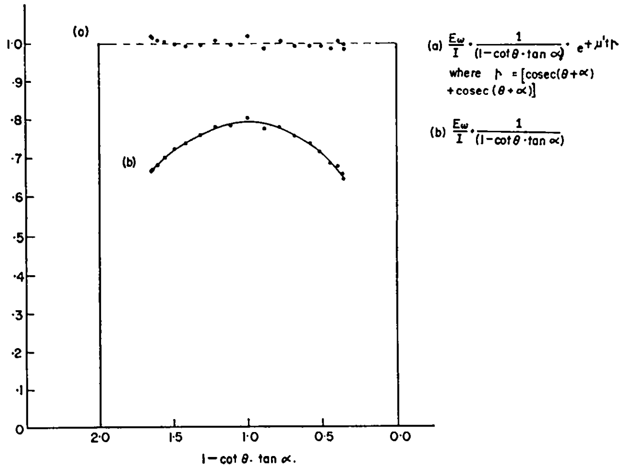

Fig. 8. Plot against $(1 - \cot\theta\,.\,\tan\alpha)$ of (*a*) $E\omega/I\,(1 - \cot\theta\,.\,\tan\alpha)^{-1}\,.\,\exp\{+\mu' t\,[\operatorname{cosec}(\theta+\alpha) + \operatorname{cosec}(\theta-\alpha)]\}$, (*b*) $E\omega/I\,(1 - \cot\theta\,.\,\tan\alpha)^{-1}$ scaled here to the same level. See Table 1.

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* If μ' is taken as the normal μ(Cu $K\alpha$) value for lithium fluoride, 32·38 cm^{-1}, then the value of t derived from $\mu t = 0{\cdot}046$ is $1{\cdot}4 \times 10^{-2}$ mm.

0·005) is shown in Fig. 9. Its greatest significance is in the low-Bragg-angle region where extinction effects are liable to interact with this factor, hence emphasizing that a direct estimate of the magnitude of this correction factor must be made before the investigation of extinction parameters is initiated. That the values of $\mu' t$ quoted above are typical is evident from our own measurements and those of Hirsch *et al.*, *e.g.* Evans, Hirsch & Kellar (1948), Gay & Hirsch (1951), Gay, Hirsch & Kellar (1952).

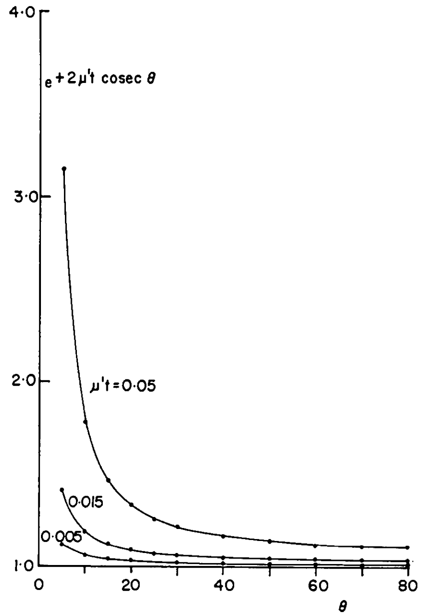

Fig. 9. Plot of exp $(+2\mu' t \operatorname{cosec} \theta)$ against θ (°) for $\mu' t=0·05$, 0·015 and 0·005.

Conclusion

From measurements on a specimen of lithium fluoride, it is shown that, for extended-face crystals with asymmetry α, the average of the two measurements at $+\alpha$ and $-\alpha$ cannot be assumed equal to that at the symmetrical position, $\alpha=0°$, as was implied by Bragg (1914).

With the measured intensities from this extended-face crystal over a range of asymmetry, $+\alpha_0$ to $-\alpha_0$, and by reference to the implications of similar studies by Hirsch and his colleagues, it has been concluded that the formula for the absorption factor given in standard texts, *e.g. International Tables for X-ray Crystallography* (1967), associated with the determination of integrated intensity, is incomplete. An additional component is required to take account of absorption associated with any surface layer due to preparative polishing or abrading procedures or its equivalent in terms of distributed protuberances. Since this component can be established experimentally, it should be mandatory for the experimentalist using an extended-face crystal to determine the magnitude of the effect on his particular specimen.

Depending on the thickness of the surface layer, the absolute scale of intensity at a given θ value will be

Table 1. *Results for* LiF

Column 2 records unscaled values of measured intensity. Column 4 gives the correction factor to normalize for effective equal scattering volume. Column 6 is the function $p=[\operatorname{cosec}(\theta+\alpha)+\operatorname{cosec}(\theta-\alpha)]$. In the last column, the figures in brackets represent the ratio of the listed value divided by the mean value 105854. For reference, and to indicate the influence of the absorption effect on the data in columns 2 and 5, the listed values are also divided by 105854 and recorded in brackets.

ϕ(°)	Integrated intensity, $E\omega/I$ Average of values at ϕ and $(180-\phi)$	α	f_v*	$\frac{E\omega}{I}\cdot\frac{1}{f_v}$	p	$f_p=\exp(+\mu' tp)$	$\frac{E\omega}{I}\cdot\frac{1}{f_v}\cdot f_p$
−90	115650 (1·093)	−15°	1·6468	70227 (0·663)	9·306	1·5344	107756 (1·018)
−80	115734 (1·093)	−14°47′	1·6369	70703 (0·668)	9·097	1·5197	107447 (1·015)
−70	115824 (1·094)	−14°8′	1·6077	72043 (0·681)	8·535	1·4808	106681 (1·008)
−60	115698 (1·093)	−13°4′	1·5601	74161 (0·701)	7·820	1·4329	106265 (1·004)
−50	114181 (1·079)	−11°36′	1·4954	76355 (0·721)	7·072	1·3844	105706 (0·999)
−40	110579 (1·045)	−9°46′	1·4157	78109 (0·738)	6·410	1·3430	104900 (0·991)
−30	106187 (1·003)	−7°38′	1·3235	80232 (0·758)	5·891	1·3113	105208 (0·994)
−20	101006 (0·954)	−5°14′	1·2211	82717 (0·781)	5·518	1·2889	106614 (1·004)
−10	92247 (0·871)	−2°40′	1·1122	82941 (0·784)	5·270	1·2743	105692 (0·998)
0	84893 (0·802)	0°	1·0000	84893 (0·802)	5·226	1·2717	107958 (1·020)
10	72490 (0·689)	2°40′	0·8878	82158 (0·776)	5·270	1·2743	104694 (0·989)
20	64330 (0·608)	5°14′	0·7789	82591 (0·780)	5·518	1·2889	106452 (1·006)
30	54254 (0·513)	7°38′	0·6765	80198 (0·758)	5·891	1·3113	105164 (0·993)
40	45719 (0·432)	9°46′	0·5843	78246 (0·739)	6·410	1·3430	105084 (0·993)
50	38256 (0·361)	11°36′	0·5046	75814 (0·716)	7·072	1·3844	104957 (0·992)
60	31983 (0·302)	13°4′	0·4399	72705 (0·687)	7·820	1·4329	104179 (0·984)
70	28115 (0·266)	14°8′	0·3923	71667 (0·677)	8·535	1·4808	106124 (1·003)
80	25256 (0·239)	14°47′	0·3631	69554 (0·657)	9·097	1·5197	105706 (0·999)
90	24086 (0·228)	15°	0·3532	68194 (0·644)	9·306	1·5344	104637 (0·989)
						Mean value	105854

* $f_v=1-\cot\theta \, . \, \tan\alpha$.

affected. Since the factor is θ-dependent, failure to take account of it may have significant influence on temperature factors and extinction parameters derived from the measurement of a series of reflexions.

With the inbuilt flexibility of modern diffractometers, there is increased interest in the potential of this classical technique to measure structure factors of high precision. Establishment of such data on an absolute scale is only possible if all correction factors are recognized, assessed and included. In the past, the influence of surface-layer absorption on structure factors derived by this procedure has been largely overlooked.

In relation to this technique, Wooster & Macdonald (1948) have drawn attention to the trend of the two limiting values of intensity – that for the perfect crystal and that for the ideally imperfect crystal – to approach one another with increasing wavelength. They concluded that it is advantageous to use longer wavelengths for the determination of accurate structure factors. This region is obviously one in which inclusion of the correction factor for surface-layer absorption is essential.

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A Classical Derivation of the Dynamical Diffraction Equation for Imperfect Crystals Based on the Ewald–Laue–Bethe Theory

BY MASAO KURIYAMA

National Bureau of Standards, Institute for Materials Research, Washington, D.C. 20234, *U.S.A.*

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The basic equation of dynamical diffraction for imperfect crystals, which has been derived previously by a general dynamical theory of diffraction, is rederived classically based on the Ewald–Laue–Bethe concept, thus completing the formulation of a 'scattering matrix' theory. It is shown in this classical derivation that a series of assumptions is required at each stage of the mathematical formulation to allow it to proceed further. These assumptions are then viewed in terms of the general dynamical theory of diffraction, and found unnecessary in the rigorous formulation. This classical formulation provides a conceptual relation between the traditional Ewald–Laue–Bethe dynamical theory and the general dynamical theory, one that has been derived with the aid of quantum-field theory.

1. Introduction

A general dynamical diffraction theory for imperfect crystals has been formulated previously by use of a quantum-field theoretical treatment of scattering problems (Ashkin & Kuriyama, 1966; Kuriyama, 1967). This theory has succeeded in rigorously deriving a fundamental equation of dynamical diffraction in the momentum representation (Kuriyama, 1970, 1972) and a basic integral equation for topography in the spatial coordinate representation (Kuriyama & Early, 1974). In addition to rigor, another virtue of this theory is that the optical conditions are automatically included in the theory (for example, Ashkin & Kuriyama, 1966; Kuriyama, 1968*a*). This is particularly important because imperfect crystals lack periodic translational invariance; diffracted beams behave differently in their intensity and angular divergence, depending upon both the location of the incident beam on the crystal and the exit locations of the diffracted beams. This property of diffracted beams has made it possible to develop a new field of diffraction topography.