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The Reflexion and Transmission of X-rays in Perfect Absorbing Crystals

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The absorption of X-rays diffracted by perfect crystal slabs is discussed in terms of the dynamical theory of X-ray diffraction for perfect absorbing crystals. This theory is presented in a form suitable for comparison with experiments. The experimental results of Borrmann are interpreted, and found to be in good quantitative agreement with the theory. Some observations by Campbell are also discussed.

Introduction

In recent years the effect of absorption on the intensities of X-rays reflected by crystals has been studied both theoretically and experimentally. Bragg reflexions (i.e. X-rays reflected off a crystal surface) and, in particular, asymmetric reflexions have been discussed previously (Hirsch & Ramachandran, 1950). For Laue reflexions (i.e. X-rays reflected through crystal slabs), the experiments of Borrmann (1941, 1950) have shown that the absorption coefficient is greatly reduced for X-rays incident at the Bragg angle. The intensities of Laue reflexions from perfect absorbing crystals have been discussed by Zachariasen (1945) on the basis of Laue's dynamical theory of X-ray diffraction. More recently, von Laue (1949) has treated this case and the transmission of X-rays incident at the Bragg angle, and has been able to show that the order of magnitude of Borrmann's results may be expected.*

The purpose of this paper is to present the theory in a form which enables a direct quantitative comparison to be made with experiment. It is possible to calculate from the theory the intensity of reflexion and transmission of a parallel monochromatic X-ray beam as a function of the angle of incidence to the reflecting planes. Experimentally, however, it is generally only possible to determine quantities related to these intensity curves, such as the integrated intensity and the position of the peak. In Borrmann's experiments (1950) a bundle of X-rays from an X-ray tube focus is allowed to fall on to a crystal slab, and the reflected and transmitted rays are recorded on a photographic plate (Fig. 1). Owing to the finite size of the focus, X-rays covering a range of angles of incidence superimpose at any point on the film. An examination of Borrmann's experimental arrangement (Borrmann, 1950) shows that the smallest angle subtended by the focus at points on the film where measurements were made was $\sim 10''$, and this small range is of the order of the angular width of reflexion. Hence the measured peak intensity is likely to be roughly proportional to the integrated intensity. (For a detailed discussion of the determination of integrated reflexions from stationary crystals reference should be made to Hirsch (1950) and to Gay, Hirsch & Kellar (1952).)

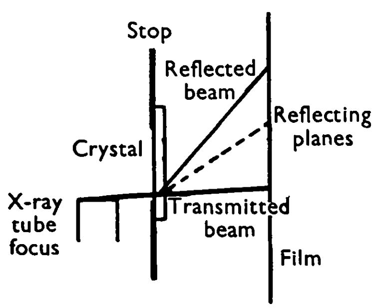


Fig. 1. Borrmann's experimental arrangement.

More recently, some experiments on Laue reflexions have been reported in which a double-crystal spectrometer was used (Campbell, 1951*a*). From these experiments the integrated intensities can be obtained, as well as the angular positions of the peaks of the reflected and transmitted beams.

It was decided, therefore, to calculate theoretically the integrated intensities of the reflected and transmitted beams when the crystal is set at the Bragg angle. This paper deals in the main with the results of these calculations and with their comparison with the experimental measurements. The agreement obtained between the theory and the experiments of Borrmann represents a direct quantitative proof of the essential correctness of the treatment of absorption according to the dynamical theory.

Notation

θ	Grazing angle of incidence on crystal planes.
θ_B	Bragg angle.
b	Ratio of the direction cosines (γ_0, γ_H) of incident and reflected beams relative to normal to surface.
α	$\equiv 2(\theta_B-\theta)\sin 2\theta_B$.

* In this paper the X-rays transmitted in the direction of reflexion and in the direction of incidence are referred to as reflected and transmitted beams respectively.

- ψ_0', ψ_0'' Real and imaginary parts of the Fourier component of index zero of 4π times the polarizability.
- ψ_H', ψ_H'' Real and imaginary parts of the Fourier component of index H of 4π times the polarizability.
- y $\equiv \{\frac{1}{2}(1-b)\psi_0'+\frac{1}{2}b\alpha\}/K|\psi_H'||b|^{\frac{1}{2}}$.
- g $\equiv \frac{1}{2}(1-b)\psi_0''/K|\psi_H'||b|^{\frac{1}{2}}$.
- k $\equiv \psi_H''/\psi_H'$.
- A $\equiv \pi K|\psi_H'|t_0/\lambda|\gamma_0\gamma_H|^{\frac{1}{2}}$.
- t_0 Thickness of crystal slab.
- t $\equiv \frac{1}{2}(1/\gamma_0+1/\gamma_H)t_0$.
- μ_0 Linear absorption coefficient.
- λ Wavelength of X-rays.
- K Polarization factor; $K=1$ for normal component (K_1) and $K=|\cos 2\theta|$ for parallel component (K_2).
- I_0 Intensity (energy per unit area) of the incident parallel and monochromatic beam.
- I_H Intensity of reflected beam of index H.
- I_T Intensity of transmitted beam.
- R_H^y Integrated intensity of reflected beam in y units of angle.
- R_T^y Integrated intensity of transmitted beam in y units of angle.

General theory

The fundamental equation of the dynamical theory is the equation of self-consistency of the wavefields inside the crystal (Zachariasen, 1945, see equation [3·110]). This equation, together with the boundary conditions, leads to expressions for the intensity of a parallel monochromatic X-ray beam reflected and transmitted by a crystal slab (equations [3·130], [3·131]). After some algebraic computation, one finds

$$\frac{I_H}{I_0} = |b|\,\frac{|q|}{|q+z^2|}\,e^{-\mu_0 t}(\sin^2 av+\sinh^2 a\omega)\,, \qquad (1)$$

$$\begin{aligned}\frac{I_T}{I_0} = \frac{e^{-\mu_0 t}}{|q+z^2|}\,\{&|q+z^2|+(|q+z^2|+|z|^2)\sinh^2 a\omega\\ &-(|q+z^2|-|z|^2)\sin^2 av\\ &\pm\tfrac{1}{2}|(|q+z^2|+|z|^2)^2-|q|^2|^{\frac{1}{2}}\sinh 2a\omega\\ &\pm\tfrac{1}{2}|(|q+z^2|-|z|^2)^2-|q|^2|^{\frac{1}{2}}\sin 2av\}\,, \qquad (2)\end{aligned}$$

where

$$q = K^2 b\psi_H\psi_{\bar{H}}\,,$$
$$z = \tfrac{1}{2}(1-b)\psi_0+\tfrac{1}{2}b\alpha\,,$$
$$a = \pi t_0/\lambda\gamma_0\,,$$
$$v+i\omega = (q+z^2)^{\frac{1}{2}}\,.$$

For a moderately strong reflexion $av \sim \pi 10^3 t_0$; since t_0 is expected to vary over a range of 10^{-3} cm., av will vary by π and hence an average must be taken. Equations (1), (2) then reduce to

$$\frac{I_H}{I_0} = \frac{1}{2}\,\frac{|b||q|}{|q+z^2|}\,e^{-\mu_0 t}\cosh 2a\omega\,, \qquad (3)$$

and

$$\begin{aligned}\frac{I_T}{I_0} = \frac{1}{2}\,\frac{e^{-\mu_0 t}}{|q+z^2|}\,\{&(|q+z^2|+|z|^2)\cosh 2a\omega\\ &\pm|(|q+z^2|+|z|^2)^2-|q|^2|^{\frac{1}{2}}\sinh 2a\omega\}\,. \qquad (4)\end{aligned}$$

The assumption is now made that the crystal possesses an inversion centre. Then, defining y, g, k, A as in the notation, equations (3), (4) transform to

$$\frac{I_H}{I_0} = \frac{1}{2}\,\frac{(1+k^2)e^{-\mu_0 t}}{[(1+y^2-g^2-k^2)^2+4(k+gy)^2]^{\frac{1}{2}}}\cosh 2a\omega\,, \qquad (5)$$

$$\frac{I_T}{I_0} = \frac{1}{2}\,\frac{(1+k^2)e^{-\mu_0 t}}{[(1+y^2-g^2-k^2)^2+4(k+gy)^2]^{\frac{1}{2}}}\cosh(2a\omega\pm X)\,, \qquad (6)$$

where

$$\cosh X = \{y^2+g^2+|[(1+y^2-g^2-k^2)^2+4(k+gy)^2]^{\frac{1}{2}}|\}/(1+k^2) \qquad (7)$$

and

$$2a\omega = \sqrt{2}\,A\{-(1+y^2-g^2-k^2)+|[(1+y^2-g^2-k^2)^2+4(k+gy)^2]^{\frac{1}{2}}|\}^{\frac{1}{2}}\,. \qquad (8)$$

In equation (6) the sign of X should be changed at $y=-gk$. These equations permit the explicit computation of the diffraction patterns as a function of y. These are related to the patterns as a function of the glancing angle θ through the definition of y (see notation). The shape of the curves depends only on k, g, i.e. quantities proportional to the ratio of the imaginary and real parts of the scattering factors, and on A, which is proportional to the structure factor and the thickness of the crystal. In general the curves are asymmetric.

The fuller discussion of these equations will now be confined to the case of symmetric Laue reflexions (Fig. 2). For these $b=1$ and therefore $g=0$. The

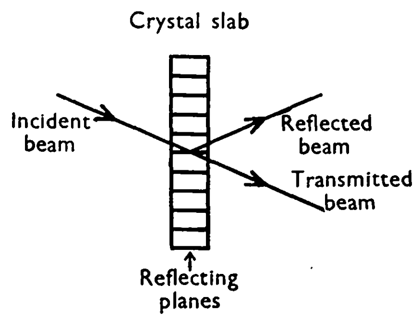


Fig. 2. Symmetrical Laue reflexion.

conclusions reached will also apply to reflexions of small degree of asymmetry for which g is small and can be neglected. Thus the results are applicable to the experiments of Borrmann (1950) in which the degree of asymmetry was small. For this case it is at once apparent that I_H/I_0 is symmetrical about the maximum at $y=0$; I_T/I_0 however, is not symmetrical.

Reflexion and transmission at $y = 0$

The influence of absorption may be discussed conveniently by considering I_H and I_T at $y = 0$. Then $\cosh X = 1$, and $2a\omega = 2Ak$, and equations (5), (6) reduce to

$$\frac{I_H}{I_0} = \frac{I_T}{I_0} = \tfrac{1}{2} e^{-\mu_0 t_0/\gamma_0} \cosh 2Ak\,. \tag{9}$$

Now

$$2Ak = \frac{\mu_0 t_0}{\gamma_0} K \frac{\psi''_H}{\psi''_0}\,;$$

since the quantities ψ are proportional to the structure factors F (see Zachariasen, 1945, equation [3·95]) this may be written in the more usual notation

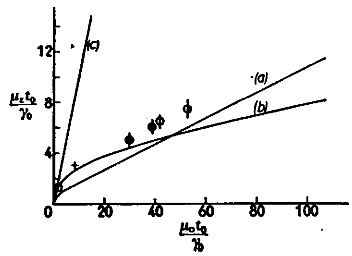
$$2Ak = \frac{\mu_0 t_0}{\gamma_0} K \frac{F''_H}{F''_0}\,, \tag{10}$$

where F''_H, F''_0 are the imaginary parts of the structure factors for the reflected and transmitted beams. As the assumption has been made that the crystal possesses an inversion centre, the imaginary parts of the structure factors are due to the imaginary parts of the atomic scattering factors which take into account absorption. Since the absorption is generally mainly due to the K shells whose dimensions are small compared with the X-ray wavelengths, KF''_H/F''_0 can be of the order of unity, and hence it is clear that for large values of $\mu_0 t_0/\gamma_0$ the effective absorption may be reduced considerably. In the case of zero absorption $I_H/I_0 = I_T/I_0 = \frac{1}{2}$, and one may define an effective absorption coefficient μ_E such that for absorbing crystals

$$\frac{I_H}{I_0} = \frac{I_T}{I_0} = \tfrac{1}{2} e^{-\mu_E t_0/\gamma_0}\,.$$

It follows from (9), (10) that the absorption is different for the two directions of polarization. The order of magnitude of the effect may, however, be seen by taking $KF''_H/F''_0 = 0{\cdot}9$, which is an average value over the two directions of polarization for a cleavage reflexion from calcite at $\lambda = 1{\cdot}54$ Å. Curve (*a*) in Fig. 3 represents $\mu_E t_0/\gamma_0$ plotted against $\mu_0 t_0/\gamma_0$ for this case. The drastic reduction of absorption is apparent. It is easy to show that for large values of $\mu_0 t_0/\gamma_0$ a limiting absorption coefficient is reached, and its value is $\mu_L = \mu_0(1 - KF''_H/F''_0)$. Taking $\mu_0 = 205$ cm.$^{-1}$ for calcite at $\lambda = 1{\cdot}54$ Å, $\mu_L = 20{\cdot}5$ cm.$^{-1}$.

Although these considerations help to obtain an idea of the orders of magnitude involved, it is doubtful if any experimental method can give the value of I_H/I_0 or I_T/I_0 at $y = 0$.



○ Cu $K\alpha$ } Borrmann's experimental points; the vertical lines
● Cu $K\beta$ } give an estimate of the experimental accuracy
+ Cu $K\alpha$ Campbell's experimental result.

Fig. 3. Theoretical curves and Borrmann's experimental values of the effective absorption coefficient. (*a*) Theoretical curve of the effective absorption of the reflected and transmitted beams at $y = 0$, assuming $KF''_H/F''_0 = 0{\cdot}9$. (*b*) Theoretical curve of the effective absorption of the integrated intensity for the symmetric Laue reflexion from the cleavage planes of calcite, using unpolarised Cu $K\alpha$ or $K\beta$ radiation. (*c*) Theoretical curve of the absorption for a mosaic crystal; $\mu_E = \mu_0$.

Integrated intensities

Owing to the complexity of equations (5) and (6), direct integration is not possible and graphical methods have to be used. In all practical cases k is small (usually $< 0{\cdot}1$) and under these conditions the equations simplify to

$$\frac{I_H}{I_0} = \tfrac{1}{2} \frac{e^{-\mu_0 t_0/\gamma_0}}{(1+y^2)} \cosh \frac{2Ak}{(1+y^2)^{\frac{1}{2}}} \tag{11}$$

and

$$\frac{I_T}{I_0} = \tfrac{1}{2} \frac{e^{-\mu_0 t_0/\gamma_0}}{(1+y^2)} \cosh \left(\frac{2Ak}{(1+y^2)^{\frac{1}{2}}} \pm X \right), \tag{12}$$

where $\cosh X = 1 + 2y^2$. (The change of sign in (12) occurs at $y = 0$ for symmetric Laue reflexions.) For

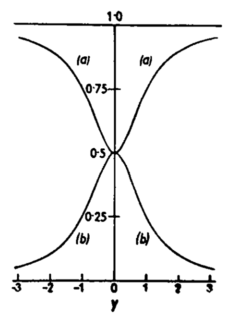


Fig. 4. Intensity curves for transmitted and reflected beams.

(*a*) I_T/I_0 }
(*b*) I_H/I_0 } against y, for $Ak = 0$.

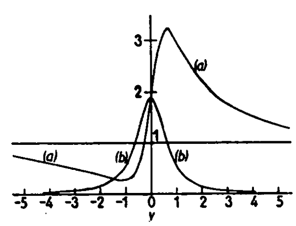


Fig. 5. Intensity curves for transmitted and reflected beams.

(*a*) $\frac{I_T}{I_0} e^{\mu_0 t_0/\gamma_0}$ }
(*b*) $\frac{I_H}{I_0} e^{\mu_0 t_0/\gamma_0}$ } against y, for $Ak = 1$.

large values of y, $I_H/I_0 \to 0$ and $I_T/I_0 \to e^{-\mu_0 t_0/\gamma_0}$ as expected. Figs. 4, 5 and 6 represent curves of $e^{\mu_0 t_0/\gamma_0} . I_H/I_0$ and $e^{\mu_0 t_0/\gamma_0} . I_T/I_0$ for various values of Ak. These curves show clearly how with increasing Ak the 'extinction line' is replaced by an increase

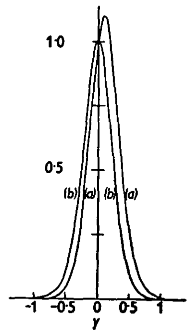


Fig. 6. Intensity curves for transmitted and reflected beams.

$$\left.\begin{array}{ll}(a) & \dfrac{I_T}{I_0}\cdot\dfrac{2}{\cosh 20}\cdot e^{\mu_0 t_0/\gamma_0} \\ (b) & \dfrac{I_H}{I_0}\cdot\dfrac{2}{\cosh 20}\cdot e^{\mu_0 t_0/\gamma_0}\end{array}\right\} \text{ against } y, \text{ for } Ak=10.$$

of intensity due to reduced true absorption. Traces of the asymmetry of the transmitted beam, and in particular the decrease and subsequent increase of intensities, have been reported by Borrmann (1941) and are also apparent in the figures published by Campbell (1951*a*).

The areas under the curves in Figs. 4, 5 og 6 give the integrated intensities on the y scale. The measured integrated intensities on the glancing-angle scale θ are equal to these quantities multiplied by the factor

$$\frac{K|\psi'_H|}{|b|^{\frac{1}{2}}\sin 2\theta_B}$$

(c.f. Zachariasen, 1945, p. 126). The curves of I_H/I_0 were integrated graphically. For the curves of I_T/I_0 the following procedure was adopted. The mean of the ordinates for positive and negative values of y is

$$\frac{\overline{I_T}}{I_0} = \tfrac{1}{2}e^{-\mu_0 t_0/\gamma_0}\frac{(1+2y^2)}{(1+y^2)}\cosh\frac{2Ak}{(1+y^2)^{\frac{1}{2}}} .$$

The area under this curve is equal to that under I_T/I_0. Then

$$\frac{\overline{I_T}}{I_0}+\frac{I_H}{I_0} = e^{-\mu_0 t_0/\gamma_0}\cosh\frac{2Ak}{(1+y^2)^{\frac{1}{2}}} .$$

The function

$$\left(\cosh\frac{2Ak}{(1+y^2)^{\frac{1}{2}}}-1\right)$$

was plotted and integrated for various values of Ak; from the results it was possible to obtain

$$\int\left(\frac{\overline{I_T}}{I_0}e^{+\mu_0 t_0/\gamma_0}-1\right)dy \equiv E_T .$$

As y is varied, $R_T^y = E_T e^{-\mu_0 t_0/\gamma_0}$ is equal to the intensity transmitted above the level of the 'background' at large values of y. Experimentally one can determine the total intensity transmitted above the level of the 'background' at large values of θ, i.e. the quantity

$$\frac{K|\psi'_H|}{|b|^{\frac{1}{2}}\sin 2\theta_B}E_T e^{-\mu_0 t_0/\gamma_0} .$$

E_T and the corresponding quantity

$$E_R\left(=\int\frac{I_H}{I_0}e^{+\mu_0 t_0/\gamma_0}dy\right)$$

are plotted in Fig. 7 as a function of Ak. These are monotonically increasing functions of Ak, indicating

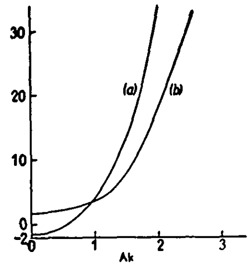


Fig. 7. Integrated intensities.

$$\left.\begin{array}{ll}(a) & E_T \\ (b) & E_R\end{array}\right\} \text{ against } Ak.$$

the decrease of the effective absorption coefficient. For calculation purposes the quantities $E_T/\cosh 2Ak$ and $E_R/\cosh 2Ak$ are useful and are shown in Fig. 8. For small absorption (i.e. small Ak) E_T is negative,

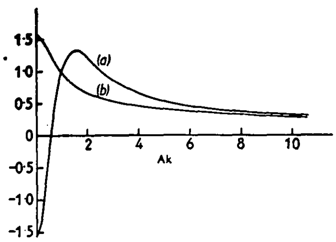


Fig. 8. Integrated intensities.

$$\left.\begin{array}{ll}(a) & E_T/\cosh 2Ak \\ (b) & E_R/\cosh 2Ak\end{array}\right\} \text{ against } Ak.$$

indicating extinction. The 'reversal' of the line occurs when

$$2Ak = \frac{\mu_0 t_0}{\gamma_0}K\frac{F''_H}{F''_0} \sim 1 .$$

Since $KF''_H/F''_0 < 1$, $\mu_0 t_0/\gamma_0 > 1$, i.e. 'reversal' occurs only when absorption becomes really important. Although $E_T > E_H$ for values of $Ak > 1$, for very large values of $Ak, E_T \to E_H$. This can be derived directly from the equations. For large Ak,

$$\cosh \frac{2Ak}{(1+y^2)^{\frac{1}{2}}}$$

varies much faster than $(1+y^2)$ or $(1+2y^2)$; hence

$$\frac{I_H}{I_0} = \frac{I_T}{I_0} = \tfrac{1}{4} e^{-\mu_0 t_0/\gamma_0} e^{2Ak/(1+y^2)^{\frac{1}{2}}} \doteqdot \tfrac{1}{4} e^{-\mu_0 t_0/\gamma_0} e^{2Ak} e^{-Aky^2} .$$

This can be integrated to give

$$\frac{E_R}{\cosh 2Ak} = \frac{E_T}{\cosh 2Ak} = \tfrac{1}{2}(\pi/Ak)^{\frac{1}{2}} .$$

This relation is accurate to $\sim 10\%$ for $Ak > 10$.

The physical explanation of these results is that in a perfect crystal multiple reflexions take place and that the resulting waves in the direction of incidence and reflexion in the crystal interfere to produce a stationary wave system. The nodal planes of this system are parallel to the reflecting lattice planes. If the nodal planes coincide with planes of absorbing atoms, the absorption will be a minimum. For the waves satisfying this condition the absorption is reduced. The 'reversal' of the extinction line is therefore due to a decrease of the true absorption, and does not contradict the existence of the phenomenon of extinction. This also explains why reversal takes place only when absorption has become important in the crystal. A full discussion of the physical interpretation has been given by Borrmann (1950).

Comparison with experiments

In most of the experiments cleavage reflexions from calcite were examined with Cu $K\alpha$ and $K\beta$ radiations (Borrmann, 1950; Campbell, 1951*a*). The absorption coefficients for these two wavelengths are 205 cm.$^{-1}$ and 151 cm.$^{-1}$ respectively. The values of F''_H and F''_0 required in the theory have been calculated by Zachariasen (1945, p. 144) for this reflexion for Cu $K\alpha$ radiation, using Hönl's (1933 *a*, *b*) formula for the imaginary part of the scattering factor. For the Cu $K\alpha$ radiation F''_H/F''_0 is found to be 0·9575. A similar calculation for Cu $K\beta$ radiation showed F''_H/F''_0 to be very nearly equal to this value.

Effective absorption coefficient

In order to compare the calculated values of E_T and E_R with Borrmann's results it is necessary to define an effective absorption coefficient as follows. For each direction of polarisation

$$R^y_H = E_R e^{-\mu_0 t_0/\gamma_0} = \left(\frac{E_R}{\cosh 2Ak}\right) (e^{-\mu_0 t_0/\gamma_0} \cosh 2Ak) .$$

To a first approximation $E_R/\cosh 2Ak$ varies slowly with Ak. Therefore, for unpolarised radiation, which is the case in Borrmann's experiments,

$$R^y_H = \left(\frac{E_R}{\cosh 2Ak}\right) e^{-\mu_0 t_0/\gamma_0} \cosh m \cosh d ,$$

where

$$m = \frac{K_1+K_2}{2} \cdot \frac{F''_H}{F''_0} \cdot \frac{\mu_0 t_0}{\gamma_0} ,$$

$$d = \frac{K_1-K_2}{2} \cdot \frac{F''_H}{F''_0} \cdot \frac{\mu_0 t_0}{\gamma_0} .$$

The effective absorption coefficient μ_E is defined such that

$$R^y_H = R^y_H(Ak = 0) e^{-\mu_E t_0/\gamma_0} = \tfrac{1}{2}\pi e^{-\mu_E t_0/\gamma_0} ,$$

or

$$e^{-\mu_E t_0/\gamma_0} = \frac{2}{\pi} \left(\frac{E_R}{\cosh 2Ak}\right) e^{-\mu_0 t_0/\gamma_0} \cosh m \cosh d .$$

For very large values of Ak this reduces to

$$e^{-\mu_E t_0/\gamma_0} = \frac{1}{4} \frac{1}{(\pi Ak)^{\frac{1}{2}}} \exp\left[-\frac{\mu_0 t_0}{\gamma_0}\left(1-\frac{F''_H}{F''_0}\right)\right] ,$$

giving a limiting absorption coefficient

$$\mu_L = \mu_0 \left(1-\frac{F''_H}{F''_0}\right) .$$

μ_E has been calculated for the cleavage reflexion from calcite for Cu $K\alpha$ radiation as a function of $\mu_0 t_0/\gamma_0$, and the curve is shown in Fig. 3(*b*). The limiting absorption coefficient is found to be $= 8·7$ cm.$^{-1}$. Borrmann determined experimentally the effective absorption coefficient as a function of $\mu_0 t_0$; in the experiments, however, $\gamma_0 \doteqdot 1$ so that his points have been transferred directly to Fig. 3. He found that the points for Cu $K\alpha$ and Cu $K\beta$ radiation followed the same curve. This is expected from the equality of F''_H/F''_0 (see above). Although the experimental points are somewhat above the theoretical curve, the agreement is excellent and may be regarded as a satisfactory quantitative test of the effect of absorption in the theory. The slight deviation of the experimental points may be due either to small imperfections or to the temperature movement of the atoms. For comparison we have drawn the curve (*c*) $\mu_E = \mu_0$, which corresponds to the absorption coefficient in a mosaic crystal.

The limiting absorption coefficient is rather lower than Borrmann's value between 15 and 19 cm.$^{-1}$. This is to be expected since the discrepancy would be worse at the largest values of $\mu_0 t_0/\gamma_0$. Nevertheless the agreement in the order of magnitude is encouraging.

Campbell (1951 *a*, *b*) has measured the intensities transmitted and reflected through slabs of several different crystals, using the symmetric Laue arrangement and crystal-monochromatized radiation. Increases in intensity of the transmitted beam were observed in several cases, but only one etched specimen of calcite can be regarded as sufficiently perfect to allow comparison with the theory. From Campbell's* intensity curves for this crystal (0·40 mm. thick, $10\bar{1}1$ reflexion, Cu $K\alpha$ radiation, $\mu_0 t_0/\gamma_0=8{\cdot}45$, $A=3{\cdot}8$) estimates of the integrated intensities could be made. These were found to be equal to 1·7 and 1·3 microradians for the transmitted and reflected beams respectively. The corresponding values of $\mu_E t_0/\gamma_0$ were then calculated and found to be 2·7 and 3·0 respectively. The latter point is shown on Fig. 3; the agreement with the predicted value is again satisfactory.

It should be emphasised here that this theory applies only to perfect crystals. Ideally imperfect crystals have a normal absorption coefficient μ_0. Partially imperfect crystals would be expected to exhibit an intermediate effect, which might be further complicated through secondary extinction. The influence of perfection on the effective absorption has been shown experimentally by Borrmann (1941) and is also apparent from Campbell's (1951*a*) results on etched and ground slabs of calcite. This latter author has also reported a small increase in the intensity transmitted through mica, and no increase for a crystal of hexamethylenetetramine. As both these crystals were imperfect, no definite conclusions can be reached. It is interesting to observe, however, that the absorption coefficient for the organic crystal is very small (about 6·2 cm.$^{-1}$ for Cu $K\beta$ radiation). The value of Ak for the 200 reflexion from a crystal 2 mm. thick (unpublished information from Dr Campbell) is only 0·12, and it is clear from Fig. 8 that such a crystal, if perfect, should show the extinction effect.

Equality of R_H^y and R_0^y

Both Borrmann and Campbell have reported that the intensities of the reflected and transmitted beams are sometimes nearly equal. The crystals used had a thickness of 1 mm. or more. For a plate 1 mm. thick, and Cu $K\alpha$ radiation

$$Ak=\frac{1}{2}\frac{\mu_0 t_0}{\gamma_0}\cdot K\frac{F_H''}{F_0''}=\begin{cases}10 \text{ for normal polarization,}\\ 8{\cdot}8 \text{ for parallel polarization.}\end{cases}$$

For Cu $K\beta$ radiation the corresponding values of Ak are 7·4 and 6·6. From Fig. 8 it is clear that for these values of Ak, $E_T \doteqdot E_R$, and hence the experimental results are explained.

Position of peak intensity

Besides the integrated intensity, the peak intensity can be determined experimentally. The maximum of the reflected beam occurs at $y=0$. The peak of the transmitted beam, however, occurs at finite values of y. Now

$$\frac{I_T}{I_0}=\frac{1}{2}\frac{e^{-\mu_0 t_0/\gamma_0}}{(1+y^2)}\cosh\left(\frac{2Ak}{(1+y^2)^{\frac{1}{2}}}\pm X\right);$$

for large values of Ak,

$$\cosh\left\{\frac{2Ak}{(1+y^2)^{\frac{1}{2}}}\pm X\right\}$$

varies much faster than $(1+y^2)$. The maximum and minimum values of I_T/I_0 can then be found to a good approximation by differentiation of

$$\left\{\frac{2Ak}{(1+y^2)^{\frac{1}{2}}}\pm X\right\}.$$

This leads to the co-ordinate of the peak position y_P, given by

$$y_P=\tfrac{1}{2}\{Ak-(A^2k^2-4)^{\frac{1}{2}}\}.$$

In Campbell's experiments on calcite (1951*b*), the mean value of Ak is $\sim 3{\cdot}8$. Hence $y_P=0{\cdot}29$; and the angular deviation from the Bragg angle is found to be $\sim 1''$. The curves of Campbell show a relative angular deviation of about 6″. Dr Campbell has pointed out (private communication) that this large deviation is probably due to the non-coincidence of the axis of rocking and the normal to the plane of incidence in his geometrical arrangement.

Conclusions

This paper shows how the dynamical theory of X-ray diffraction for perfect absorbing crystals may be presented in a form suitable for comparison with experiments. An interpretation of Borrmann's and Campbell's experimental results has lead to good quantitative agreement with this theory.

References

Borrmann, G. (1941). *Phys. Z.* **42**, 157.
Borrmann, G. (1950). *Z. Phys.* **127**, 297.
Campbell, H. N. (1951*a*). *Acta Cryst.* **4**, 180.
Campbell, H. N. (1951*b*). *J. Appl. Phys.* **22**, 1139.
Gay, P., Hirsch, P. B. & Kellar, J. N. (1952). *Acta Cryst.* **5**, 7.
Hirsch, P. B. (1950). Ph.D. Dissertation, University of Cambridge.
Hirsch, P. B. & Ramachandran, G. N. (1950). *Acta Cryst.* **3**, 187.
Hönl, H. (1933*a*). *Z. Phys.* **84**, 1.
Hönl, H. (1933*b*). *Ann. Phys., Lpz.* **18**, 625.
Laue, M. von (1949). *Acta Cryst.* **2**, 106.
Zachariasen, W. H. (1945). *Theory of X-ray Diffraction in Crystals.* New York: Wiley.

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