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X-RAY ANTI-REFLECTIONS IN CRYSTALS

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1. INTRODUCTION

THIS paper deals with the theory of some interesting phenomena which are observed in the transmitted X-ray beam when a Bragg reflection takes place in a crystal. Obviously, if the crystal is non-absorbing, then the whole of the incident energy must be transmitted in the absence of the Bragg reflection and when a reflection occurs, the energy which is reflected will manifest itself as a reduction in the intensity of the transmitted beam. Thus, the reflected and transmitted intensities would be complementary, so that if R and T are the reflection and transmission coefficients, then

$$R + T = 1. \tag{1}$$

If the crystal is absorbing, we have one more mechanism whereby energy may be abstracted from the incident beam. If A is the fraction of the incident intensity removed in this way, we have from *a priori* considerations, the following equation:

$$R + T + A = 1 \text{ or } R + T = 1 - A = T_0 \text{ (say)} \tag{2}$$

This means that T is always less than or equal to T_0, and near the Bragg reflection, when R has an appreciable value, there should be a reduction in the transmitted intensity.

The foregoing deduction is, however, based on the idea that absorption and reflection are independent processes. However, if one supposes that the two are interrelated and that the absorption coefficient can itself be modified by the presence of an interference maximum, then conditions may be different. Thus, if the effective absorption coefficient is reduced for directions of incidence close to the Bragg angle, then the quantity A in Eqn. (2) would itself be reduced and one cannot conclude, without further calculations, whether the transmission would effectively decrease or increase. It is conceivable that the decrease in absorption coefficient would be such that the consequent increase in the transmited intensity may be larger than the decrease due to part of the energy being reflected. In such a case, one may expect a peak in the transmitted beam near the Bragg reflection rather than a dip. In fact, such a result has been observed by Campbell (1951) using perfect calcite crystals. He found that the peak of the transmitted intensity may even be several hundred times as large as T_0. The name "anti-reflection" is suggested for this phenomenon. As is evident from the above discussion, such a phenomenon can be expected only with an absorbing crystal. If there is no absorption, Eqn. (1) would be rigorously valid and there would be always a diminution in T near a Bragg reflection. Also, the greater the value of A, *i.e.*, the thicker the crystal, the more striking would be the intensity changes produced by a small alteration in the absorption coefficient, and consequently the more prominent would be the anti-reflection peak.

These qualitative arguments are borne out by the detailed theory given below. It is based on the well-known dynamical theory of Ewald (1916). In particular, the development of the theory due to Laue (1949) forms a proper starting point for the discussion in this paper. Compact expressions have been derived for T and R, both in the so-called "Laue" and "Bragg" cases, and these have been numerically worked out in the former case. They show clearly that, for increasing thicknesses of the crystal, the transmission curve slowly alters its form from a minimum to a sharp maximum near the Bragg reflection.

2. PREVIOUS LITERATURE

On the experimental side, the subject goes back to an interesting observation made by Rutherford and Andrade (1914) during their determinations of γ-ray wavelengths using crystal diffraction. They observed in general a diminution in the intensity of the transmitted beam when a diffracted beam occurred. However, this diminution was not observed when a good perfect crystal was chosen for the experiment. In continuation of this experiment, Borrmann (1941) allowed a divergent beam of X-rays to fall on a crystal plate of quartz (0.2 mm. thick) and found lines in the transmitted beam where the transmission was appreciably reduced. However, when he chose a perfect crystal, as evidenced by the sharpness of the X-ray reflection, he found that the lines exhibited a "*Helldunkelstruktur*", *i.e.*, adjoining areas having an intensity larger and smaller than the general background. The occurrence of a transmitted beam of intensity larger than T_0 is particularly noteworthy.

Lonsdale (1947) made similar studies with a number of crystals and confirmed Rutherford and Andrade's observation. She found that the deficiency lines in the transmitted beam were imperceptible with a perfect crystal, while they became clearer with increasing degree of mosaicity. She did not make a critical study of the distribution of intensity of these lines.

Making use of the dynamical theory of X-ray diffraction, Laue (1949) has worked out the theory of the transmission of X-rays when interference takes place. In particular, he considered the so-called "Laue case", *i.e.*, when both the incident and diffracted beams emerge from the back surface of the crystal plate. Using his formulæ he also calculated numerically the angular distribution of intensity of the reflected and transmitted beams in a few particular cases. These are similar to those observed by Borrmann (1941), although no quantitative comparison can be made.

More recently, Campbell (1951 *a*, *b*) studied the phenomenon quantitatively, using Geiger-Müller counters. The experiments were performed with a monochromatised beam of Cu Kα having a small angle of divergence of the order of 15 seconds of arc. Symmetrical "Laue" reflections were obtained from the crystal under study and both the reflected and the transmitted intensities were measured simultaneously for different settings near the Bragg reflection by means of two Geiger counters. Sharp *maxima* were found *both* in the reflected and the transmitted beams with perfect crystals. With an imperfect crystal, the increase was imperceptible, but there was no decrease. Campbell has stated in his paper (1951 *b*) that the sharp maxima in the transmitted beam do not correspond to the curves given in Laue's paper (1949) and that his results are therefore inexplicable on this theory. However, the conditions of his experiment are different from those assumed in the theory and when the proper conditions are incorporated in the theory, it leads to sharp maxima, as is shown below.

3. NOTATION

The notation follows mainly Laue's symbology (1949), although a number of new symbols are used. Zachariasen (1945) has also given an account of the dynamical theory and his notation has been adopted in certain cases. The symbols within brackets are the equivalents in Zachariasen's notation of those used here.

λ	Wavelength of the X-rays in vacuum	(λ_0)
k	$(= 1/\lambda)$, length of the wave-vector in vacuum	(k_0)
h	Index (subscript) denoting a particular X-ray reflection (This index may be omitted when there is no confusion).	(H)
θ	Angle of incidence	(θ)
θ_G	Geometrical Bragg angle	(θ_B)
θ_B	Bragg angle, allowing for refraction	
μ	Linear absorption coefficient (in the absence of Bragg reflection)	(μ_0)

D	Thickness of the crystal	(t)
C	Polarisation factor, $= 1$ for the normal component and $= \cos 2\theta$ for the parallel component	(K)
γ_0 γ_h	Cosines of the angles made by the incident and reflected beams respectively with the normal to the surface	(γ_0) (γ_H)
χ_0 χ_h	Fourier components of order 0 and h in the triple Fourier expansion of $4\pi\alpha$, where α is the polarisability	(ψ_0) (ψ_H)
χ_{hr} χ_{hi}	Real and imaginary parts of $\chi_h : \chi_h = \chi_{hr} + i\chi_{hi}$	$(\psi_H{}')$ $(\psi_H{}'')$
$\mathbf{D}_0$ $\mathbf{D}_h$	Electric vectors of the diffracted waves of order 0 and h	$(\bar{D}_0)$ $(\bar{D}_H)$
D_0 D_h	Magnitudes of $\mathbf{D}_0$, $\mathbf{D}_h$	(D_0) (D_H)
$\mathbf{z}$	Unit vector, normal to the surface, directed inside the crystal	$(\bar{n})$
$\mathbf{R}_0$ $\mathbf{R}_h$	Wave vectors, of order 0 and h inside the crystal	$(\bar{k}_0{}^B)$ $(\bar{k}_H{}^B)$
1 2	Subscripts to denote the two wave fields inside the crystal	$(')$ $('')$
a d	Superscripts, a to denote the front, and d the back surface of the crystal, *e.g.*	$(^{o})$ $(^{e})$
	$D_0{}^{(a)}$ represents the electric vector of the incident beam	
α_h	$= (\sin 2\theta_G)(\theta - \theta_G)$	$(\alpha/2)$
β_h	$= 2\alpha_h - \chi_0(1 - \gamma_h/\gamma_0)$	$(2z/b)$
β_r	Real part of β_h, $= 2\alpha_h - \chi_{0r}(1 - \gamma_h/\gamma_0)$	
y	$= \beta_r/2C\left[\frac{\gamma_h}{\gamma_0}\chi_h\chi_{\bar{h}}\right]^{\frac{1}{2}}$	(y)
R T	Reflection and transmission coefficients	
T_0	Transmission coefficient in the absence of reflection, $= \exp(-\mu D)$.	

4. DYNAMICAL THEORY OF X-RAY REFLECTION

The dynamical theory, in its most general form, seeks to determine the interaction of a crystal with an incident beam of radiation and to work out the phenomena which accompany this interaction. Here, we are interested in the case when the wavelength is of the same order as the lattice spacing of the crystal, and in particular when there is only one diffracted ray. The fundamental equations in this case are:

$$\left.\begin{aligned} \frac{R_0^2 - k^2}{R_0^2} D_0 &= \chi_0 D_0 + \chi_{\bar{h}} C D_h \\ \frac{R_h^2 - k^2}{R^2} D_h &= \chi_0 D_h + \chi_h C D_0 \end{aligned}\right\} \quad (3)$$

Putting

$$R_0 = (1 + \delta_0) k \text{ and } R_h = (1 + \delta_h) k,$$

where δ_0, $\delta_h \ll 1$, one obtains the following equation as a condition for the compatibility of the two equations in (2):

$$4\delta_0\delta_h - 2\chi_0(\delta_0 + \delta_h) + C^2\chi_h\chi_{\bar{h}} - + \chi_0^2 = 0.$$

We are specially interested in settings close to the Bragg angle. When a setting is specified, then there is a definite relation between the incident and the diffracted rays, and therefore δ_0 and δ_h are also related. Thus, the equation mentioned above becomes a quadratic in δ_0 alone (or in δ_h alone), giving two roots for δ_0. Corresponding to each value of δ_0, one obtains a value of D_h/D_0 for a particular setting and thus there are two wave fields inside the crystal, into which the incident beam is split. To calculate the transmitted or the diffracted wave outside the crystal, these two wave fields have again to be summed up on emergence from the crystal.

In the application of the dynamical theory to the X-ray reflection from a parallel crystal plate, two cases arise according as the diffracted beam emerges from the same face as, or the opposite face to, that on which X-rays are incident. These two cases are commonly referred to as the "Bragg" case and the "Laue" case respectively.[8] However, a different nomenclature is called for, since the term "Bragg reflection" occurs often in connection with this subject and should not be confused with the reflection in the Bragg case. Further, it is also common to use "Laue reflection" to mean crystal reflection of *white* X-rays and "Bragg reflection" for reflection of *monochromatic* X-rays. In view of these, the terms "surface reflection" and "internal reflection" are suggested to refer to the two cases when the reflected X-rays come out of the same surface on which the incident X-rays strike and when the reflected X-rays pass through the thickness of the crystal, respectively.

If we denote by D_{01} and D_{02} the magnitude of the electric vectors in the transmitted beam corresponding to the two wave-fields 1 and 2, and by D_{h1} and D_{h2} the corresponding quantities in the diffracted beam (of order h) then the boundary conditions in the two types of reflection will be for an internal reflection

$$D_{01} + D_{02} = D_0^{(a)};\; D_{h1} + D_{h2} = 0 \quad (4)$$

and for a surface reflection,

$$D_{01} + D_{02} = D_0^{(a)};$$

$$D_{h1} \exp\left[-2\pi i\,(\mathbf{R}_{h1}\cdot\mathbf{z})\,D\right] + D_{h2} \exp\left[-2\pi i\,(\mathbf{R}_{h2}\cdot\mathbf{z})\,D\right] = 0, \qquad (5)$$

where **z** is a unit vector along the direction of the thickness. The quantities to be determined in each case, are

for an internal reflection

$$\left.\begin{aligned} D_{01} \exp\left[-2\pi i\,(\mathbf{R}_{01}\cdot\mathbf{z})\,D\right] + D_{02} \exp\left[-2\pi i\,(\mathbf{R}_{02}\cdot\mathbf{z})\,D\right] &= D_0^{(d)} \\ D_{h1} \exp\left[-2\pi i\,(\mathbf{R}_{h1}\cdot\mathbf{z})\,D\right] + D_{h2} \exp\left[-2\pi i\,(\mathbf{R}_{h2}\cdot\mathbf{z})\,D\right] &= D_h^{(d)} \end{aligned}\right\} \qquad (6)$$

and for a surface reflection

$$\left.\begin{aligned} D_{01} \exp\left[-2\pi i\,(\mathbf{R}_{01}\cdot\mathbf{z})\,D\right] + D_{02} \exp\left[-2\pi i\,(\mathbf{R}_{02}\cdot\mathbf{z})\,D\right] &= D_0^{(d)} \\ D_{h1} + D_{h2} &= D_h^{(a)} \end{aligned}\right\} \qquad (7)$$

5. EXPRESSIONS FOR R AND T IN THE CASE OF INTERNAL REFLECTION

Laue (1949) has considered this case. The formulæ (8) and (9) given below can readily be derived from his equations. Here, they have been put in a form convenient for numerical computation. Further, the rapidly varying cosine function in Laue's formulæ have been neglected, as these only represent interference bands, which arise from interference between the two surfaces of the crystal plate. These bands would be very closely spaced, the number between two successive orders of Bragg reflection being of the order of D/λ, which is about 100,000 even with a crystal 0·01 mm. thick and even more with thicker crystals. Even a variation of the order of λ in the thickness of the crystal would obliterate them. It is therefore justifiable to neglect these fine variations of intensity and to take an average. Eqn. (8) and (9) represent in fact such an average value for the intensity.

$$R = \left|\frac{\chi_h}{\chi_{\bar h}}\right| \frac{\exp\left\{-\frac{1}{2}\left(\frac{1}{\gamma_0} + \frac{1}{\gamma_h}\right)\mu D\right\}}{2\cosh^2 v_r} \cosh 2\eta D \qquad (8)$$

$$T = \frac{\exp\left\{-\frac{1}{2}\left(\frac{1}{\gamma_0} + \frac{1}{\gamma_h}\right)\mu D\right\}}{2\cosh^2 v_r} \cosh 2\,(\eta D + v_r) \qquad (9)$$

where

$$\sinh v_r = \beta_r/2C\left[\frac{\gamma_h}{\gamma_0}\chi_h\chi_{\bar h}\right]^{\frac{1}{2}} \qquad (10)$$

and

$$\eta = \frac{\frac{1}{4}\left(\frac{1}{\gamma_0} - \frac{1}{\gamma_h}\right)\beta_r\mu}{\left(\beta_r^2 + 4C^2\frac{\gamma_h}{\gamma_0}\chi_h\chi_{\bar h}\right)^{\frac{1}{2}}} + \frac{\frac{C^2}{\gamma_0}\chi_{hr}\chi_{hi}\pi k}{\left(\beta_r^2 + 4C^2\frac{\gamma_h}{\gamma_0}\chi_h\chi_{\bar h}\right)^{\frac{1}{2}}} \qquad (11)$$

In these equations, β_r is a measure of the departure of the glancing angle θ from the Bragg angle θ_B, *i.e.*, $\beta_r = 0$ corresponds to $\theta = \theta_B$.

It is interesting to note the following deductions which readily follow from eqns. (8) and (9):

(*a*) When $|\beta_r| \gg 2C \left[\frac{\gamma_h}{\gamma_0} \chi_h \chi_{\dot{h}}\right]^{\frac{1}{2}}$, *i.e.*, for directions sufficiently remote rom the Bragg angle,

$$R = 0 \text{ and } T = \exp(-\mu D/\gamma_0) = T_0 \tag{12}$$

as should be the case. This obvious result has been particularly mentioned here, because the curves in Laue's paper may lead to an erroneous impression that T increases with β_r on one side of the maximum. His curves I and II in Figs. 2 (*a*), (*b*), (*c*) have been drawn without taking into account the $\cosh^2 v_r$ in the denominator of Eqns. (8) and (9) above. When this is also included, the above result (12) follows

(*b*) when $\beta_r = 0$

$$T = \left|\frac{\chi_{k}}{\chi_{\dot{h}}}\right| R = \tfrac{1}{2} \exp - \mu D \left[\tfrac{1}{2}\left(\frac{1}{\gamma_0} + \frac{1}{\gamma_h}\right) - \frac{C}{\sqrt{\gamma_0\gamma_h}} \frac{\chi_{hi}}{\chi_{0i}}\right]. \tag{13}$$

Thus, for a crystal obeying Friedel's Law, R = T at the peak of the reflection, as has already been pointed out by Laue.

It is interesting to note that the ratio R/T_0 depends on the ratio χ_{hi}/χ_{0i}, *i.e.*, on the ratio of the *imaginary components* of the structure factors of order *h* and zero. This ratio would correspond to the F-value, *i.e.*, the ratio of the real components, for wavelengths sufficiently far away from absorption frequencies. If this is not so, then the peak intensity of an internal reflection does not represent the structure factor of the crystal.

Since $\chi_{hi} \leqslant \chi_{0i}$ and $C \leqslant 1$, R cannot exceed the value $\frac{1}{2}$ for a symmetrical internal reflection. This is to be expected, because for a non-absorbing crystal, $R = \frac{1}{2}$ at the peak.

(*c*) For intermediate values of β_r, it is convenient to introduce the quantity $y = \sinh v_r$, so that

$$\eta = \mu \left[\tfrac{1}{4}\left(\frac{1}{\gamma_0} - \frac{1}{\gamma_h}\right) \frac{y}{\sqrt{1+y^2}} + \tfrac{1}{2} \frac{C}{\sqrt{\gamma_h\gamma_0}} \frac{\chi_{hi}}{\chi_{0i}} \frac{1}{\sqrt{1+y^2}}\right] \tag{14}$$

Also, we have

$$\cosh^2 v_r = (1 + y^2) \tag{15}$$

From the above definition, $y \,\alpha\, \beta$ and hence to $(\theta - \theta_B)$, and units of y may thus be employed as abscissæ in plotting the variation of R and T with glancing angle, as has been done by Zachariasen (1945). $y = 1$ would correspond to a value of $(\theta - \theta_B)$ equal to the half-width of the corresponding surface reflection curve if the crystal is non-absorbing (*i.e.*, for the same reflection, *h*). As is well known this is of the order of a few seconds of arc, and its magnitude can be readily calculated from θ and the structure factor, so that the *y*-unit forms a convenient unit for representing reflection curves.

6. CALCULATION OF REFLECTION AND TRANSMISSION CURVES FOR INTERNAL REFLECTIONS

Laue (1949) has plotted the variation of R and T with angle θ for the 111 and 200 reflections of rock-salt, with thicknesses of the order of 0·1 mm. and using Cu K_α radiation. He obtained curves, which exhibit variations similar to those observed by Borrmann (1941), namely, an increase and decrease of intensity compared to the background on either side of the Bragg reflection. The exponent $(\mu D/\gamma)$ is of the order of 1·0 to 2·0 and is of the same order of magnitude as that employed by Borrmann, who used quartz crystals 0·2 mm. thick and Fe K_α rays. In Campbell's experiments (1951 *b*) on the other hand, calcite crystals, 0·4 to 1·00 mm. thick were used with Cu K_α, for which $\mu D/\gamma \sim 8$ to 20. The conditions in the experiments of Campbell are not therefore comparable with those assumed in Laue's calculations, and it is not surprising that the latter do not correspond to the observations of Campbell. Consequently, the authors have plotted a series of reflection and transmission curves, with varying $(\mu D/\gamma)$, for $(10\bar{1}\cdot 1)$ reflection of calcite, when the crystal is cut with its surfaces perpendicular to the lattice planes concerned.

For convenience, we write $P = \mu D/\gamma$, and a series of curves have been plotted for values of $P = 0$, 0·5, 1·0, 1·5, 2, 3, 4, 6, 8, 20. As mentioned in the last section, the abscissæ are marked in *y*-units, $y = 1$ actually corresponding to 3·6″ of arc in this case. The relevant data required for the calculation have been taken from Zachariasen (1945) and are:

$$\mu = 183 \text{ cm.}^{-1} \qquad \gamma_0 = \gamma_h = 0\cdot 967$$

$$\chi_{0r} = -17\cdot 44 \times 10^{-6} \qquad \chi_{0i} = -0\cdot 448 \times 10^{-6}$$

$$\chi_{hr} = -8\cdot 57 \times 10^{-6} \qquad \chi_{hi} = -0\cdot 429 \times 10^{-6}$$

The curves in Figs. 1 and 2 correspond only to the normally polarised component $(C = 1)$. Since μ and γ are fixed quantities for the different curves, varying values of P correspond to varying thicknesses D, which may be readily calculated, since $\mu/\gamma = 189$.

The curve for $P = 0$ is hypothetical, for with an absorbing crystal $(\mu \neq 0)$, P can become zero only if the thickness D vanishes. Actually, eqns. (8) and (9) from which the curves have been plotted assumes that the thickness of the crystal is large enough compared with the lattice spacing. However, this particular curve may be said to correspond to the case when the crystal becomes non-absorbing, other conditions remaining the same. All the other curves relate to crystals of varying thickness D.

The following are clear from these curves. Considering first Fig. 1 (reflection), all the curves are symmetrical about the ordinate for the peak. The peak intensity steadily decreases with increasing thickness, but the decrease is far less rapid than the corresponding decrease of T_0. Thus, for $P = 0$, the peak is $0 \cdot 5$ ($T_0 = 1$); this decreases only to about $0 \cdot 23$ for $P = 2$, when the transmitted beam has dropped to $0 \cdot 135$. Thereafter the decrease in the peak intensity of the reflected beam is much less rapid. In fact for $P = 20$, for which T_0 will only have a value of the order of 10^{-9}, the peak reflection is as large as $0 \cdot 1$, *i.e.*, about a hundred million times the transmitted intensity for settings away from the Bragg reflection.

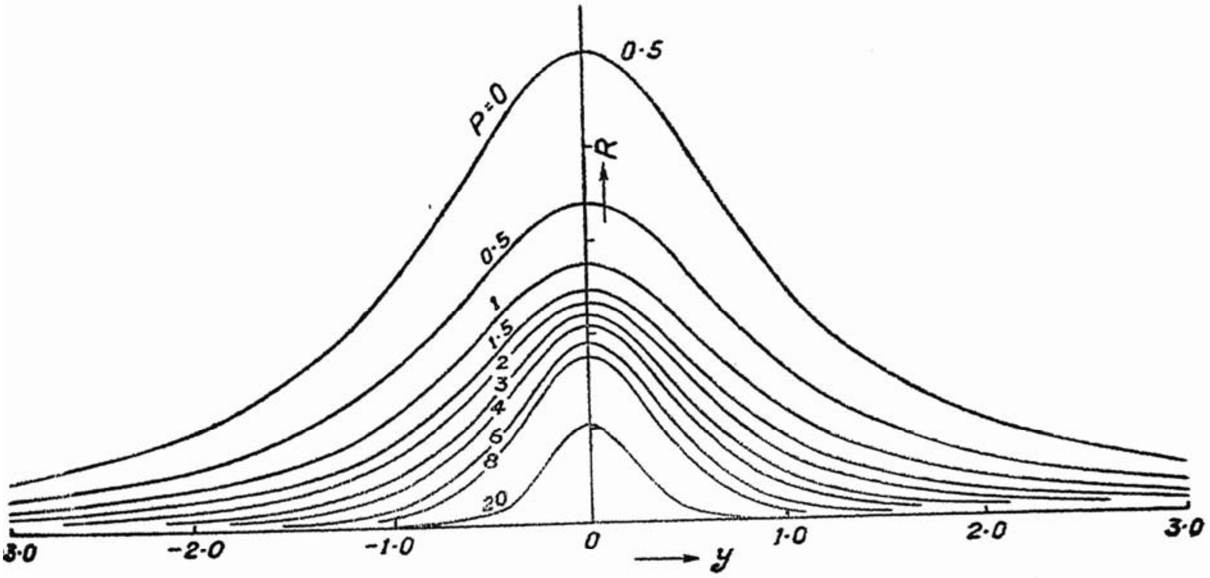

FIG. 1. Reflection curves for varying thickness of the crystal. The parameter $P = \mu D/\gamma$.

The variations in the intensity of the transmitted beam predicted by the theory is even more interesting. For $P = 0$ obviously the transmission curve (Fig. 2) is complementary to the reflection curve and exhibits only a minimum. However, for small finite values of P (*i.e.*, for small thicknesses), it exhibits both a minimum and a maximum and the intensity distribution is asymmetric about the peak of the Bragg reflection (*i.e.*, $y = 0$). On approaching the Bragg setting from the left, the transmitted intensity first becomes less than the normal value (T_0), then it rises and becomes larger

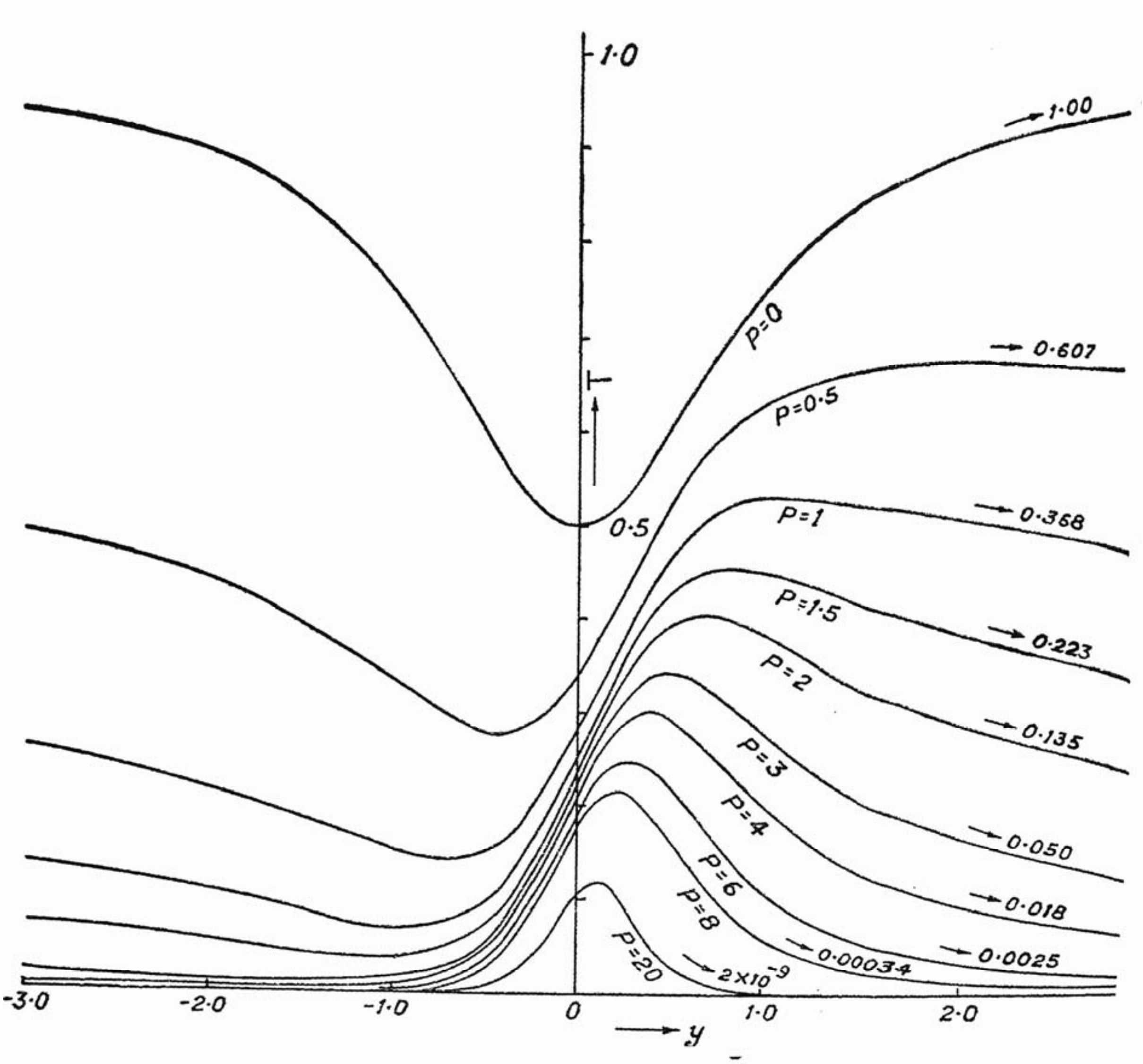

FIG. 2. Transmission curves for varying thickness of the crystal.

than the normal value, finally falling back to T_0. For small values of **P**, *i.e.*, very thin crystals, the decrease predominates, while with increasing thickness, the increase becomes larger and larger, until at $P = 2$ the increase is larger than the decrease. For still thicker crystals the minimum is imperceptible and only a peak is observed in the transmitted beam. It is interesting to note that the peak intensity of the transmitted beam is of the same order as that of the reflected beam, although the two peaks do not coincide. This is clearer from Fig. 3, which is discussed below. Thus, for P = 20, which would correspond approximately to 1 mm. of calcite, the peak value of T is several million times the value of T_0.

We shall now consider how the theory fits the observations of Campbell. For this purpose, Fig. 3 has been drawn to correspond to Fig. 6 of his paper (1951 *b*), namely, for a crystal of calcite of thickness 0·4 mm. It is obvious at once that the theory qualitatively explains his observations (*a*) that *both* the reflected and transmitted beams exhibit sharp maxima rising up to several times above the background, (*b*) that the peak intensities of the two are nearly equal to each other and (*c*) that the peaks are extremely sharp. However, quantitative agreement is not to be expected because the theoretical curve is for an incident beam of negligibly small divergence, while in the experiment, it had a divergence of the order of 15″ of arc, which is larger than the theoretical width of the reflection or transmission curves. Because of this, the observed curves would be much broader than what is predicted by theory and the peak intensity would also be lower. When these are taken into account, the agreement between theory and experiment must be considered good.

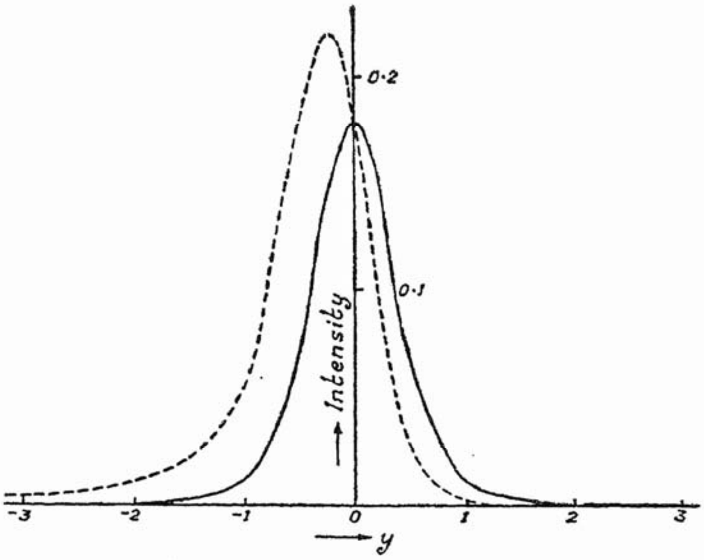

FIG. 3. Reflection (full line) and Transmission (dotted line) Curves of a crystal of calcite 0·4 mm. thick. $y = 1$ corresponds to 3·6″ of arc.

As is clear from Fig. 3, the peaks in the reflected and transmitted beams do not coincide. Campbell (1951 *b*) did observe such an effect, but he attributed it to a mis-setting of the crystal. More careful experiments should be made to verify whether such an effect is really present or not.

The curves also show that the peak in the transmitted beam is not likely to be observed unless the incident beam has a small divergence. If it has a large divergence, the effect would only be an average over a range of angles. This may lead to a net increase or decrease in the transmitted intensity over the background according to the thickness of the perfect crystal. For very thin crystals, it is a decrease and changes to an increase for thicker crystals. This explains the observation of Lonsdale (1947) that the deficiency lines observed by her with mosaic crystals became less clear and sometimes vanished with perfect crystals. She studied mostly crystals of low absorption (diamond and other organic crystals), for which P ~ 1 to 2 with a thickness of the order of a few millimetres. Consequently, if the whole crystal were perfect, there would be practically no reduction or increase in T, while if it is mosaic, a reduction would be observed. Of course, the above curves relate to calcite $10\bar{1}\cdot 1$ reflection and the conditions would be different with the crystals studied by Lonsdale (1947), but the orders of magnitude are not likely to be different. The authors have undertaken a theoretical study of the variation of R and T with various factors such as the structure factor, absorption coefficient, etc., and this would throw further light on the subject.

7. EXPRESSIONS FOR R AND T IN THE CASE OF SURFACE REFLECTION

As mentioned earlier, although Kohler (1933) has considered this case, he has made some approximations, *e.g.*, neglecting one of the two wavefields in the crystal, as it has a large attenuation coefficient. It is, however, unnecessary to make the approximation and we shall give below a brief derivation of the formulæ, both for the reflection and transmission coefficients, following closely the method and nomenclature of Laue (1949).

In the Bragg case, γ_h/γ_0 is negative and where necessary this will be denoted explicitly by writing it as $-\,|\gamma_h/\gamma_0|$.
Let

$$\beta = 2a_h - \chi_0 (1 - \gamma_h/\gamma_0)$$

Analogous to eqns. (29), (30), (31) of Laue (1949), we obtain

$$\left(\frac{D_h}{D_0}\right)_{1,2} = \left(\frac{\chi_h}{\chi_{\bar{h}}}\left|\frac{\gamma_0}{\gamma_h}\right|\right)^{\frac{1}{2}} e^{\mp u}, \tag{10}$$

where

$$\cosh u = \frac{\beta}{2C}\left[\left|\frac{\gamma_h}{\gamma_0}\right| \chi_h \chi_{\bar{h}}\right]^{\frac{1}{2}}. \tag{11}$$

We have the boundary conditions

$$D_{01} + D_{02} = D_0^{(a)};$$

$$D_{h1} \exp\left[-2\pi i\,(\mathbf{R}_{h1}\cdot \mathbf{z})\,D\right] + D_{h2} \exp\left[-2\pi i\,(\mathbf{R}_{h2}\cdot \mathbf{z})\,D\right] = 0. \tag{12}$$

nd we have to determine the quantities

$$D_{h}^{(a)} = D_{h1} + D_{h2};$$

$$\mathbf{D}_0^{(d)} = D_{01} \exp\left[-2\pi i (\mathbf{R}_{01}\cdot\mathbf{z})\,D\right] + D_{02} \exp\left[-2\pi i (\mathbf{R}_{02}\cdot\mathbf{z})\,D\right] \tag{13}$$

where $\mathbf{z}$ is a unit vector in the direction of the thickness D. If we write

$$\mathbf{R}_{01,2} = \mathbf{R}_0^{(a)} - k\delta_{1,2}\,\mathbf{z}, \tag{14}$$

where $\delta_{1,2}$ have the values [from Laue, 1949, Eqn. (21)]

$$\delta_{1,2} = -\tfrac{1}{2}\frac{\chi_0}{\gamma_0} + \frac{\beta}{4\gamma_h} \pm \frac{1}{4\gamma_h}\left[\beta^2 + 4C^2\frac{\gamma_h}{\gamma_0}\,\chi_h\chi_{\bar h}\right]^{\frac{1}{2}}. \tag{15}$$

Then, from eqns. (12), we have

$$D_{01} = \frac{\exp(u+x)}{2\sinh(u+x)}\,D_0^{(a)};\quad D_{02} = -\frac{\exp-(u+x)}{2\sinh(u+x)}\,D_0^{(a)}, \tag{16}$$

where

$$x = -\pi i k D(\delta_1 - \delta_2). \tag{17}$$

Substituting in eqns. (13), we obtain

$$\mathbf{R} = \left|\frac{\chi_h}{\chi_{\bar h}}\right|\left|\frac{\sinh x}{\sinh(u+x)}\right|^2 \tag{18}$$

$$\mathbf{T} = \left|\exp - 2\pi i k D\left(\frac{1}{\gamma_0} - \frac{\delta_1 + \delta_2}{2}\right)\right|^2 \cdot \left|\frac{\sinh u}{\sinh(u+x)}\right|^2. \tag{19}$$

Unlike the Laue case, it is not possible to put eqns. (18) and (19) in terms of real quantities alone. This is so because u (and x) may be predominantly real (*i.e.*, real part $\gg$ imaginary part) for certain values of y and predominantly imaginary for other values.*

When the reflection is symmetric, *i.e.*, it takes place from lattice planes parallel to the surface, and if Friedel's law holds (*i.e.*, $|\chi_h| = |\chi_{\bar h}|$), then eqns. (18) and (19) reduce to

$$\mathbf{R} = \left|\frac{\sinh x}{\sinh(u+x)}\right|^2 \qquad \mathrm{T} = \left|\frac{\sinh u}{\sinh(u+x)}\right|^2 \tag{20}$$

These may be compared with the corresponding expressions obtained by one of the authors (Ramachandran, 1942, 1944) for a finite parallel-sided crystal plate having n lattice planes parallel to its surface. The latter are

$$\mathbf{R} = \left|\frac{\sinh n\beta}{\sinh(\alpha + n\beta)}\right|^2 \qquad \mathrm{T} = \left|\frac{\sinh \alpha}{\sinh(\alpha + n\beta)}\right|^2. \tag{21}$$

It is clear that there is an exact correspondence between the two, and an examination of the significance of the quanitties α and $n\beta$ in eqns. (21)

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* *e. g.*, when there is no absorption, u is pure imaginary for $-1 < y < +1$ and completely real for values of y outside these limits.

shows that they are the same as u and x. This again confirms the statement made by Ramachandran (1948) that the Ewald and Darwin methods lead to identical results, in spite of their apparently very different mathematical approaches.

SUMMARY

The paper deals with the theory of an interesting phenomenon (which has been designated as "anti-reflection") that the intensity of the transmitted beam may exhibit a peak larger than the background when a Bragg reflection occurs in an absorbing crystal. The theory is based on the dynamical theory of Ewald and Laue. It comes out that the effect is due to a decrease in the effective absorption coefficient of the crystal near the Bragg reflection, and to the consequent increase in the transmitted intensity predominating over the loss of energy by reflection. The anti-reflection peak becomes more prominent, the greater the thickness of the crystal. The results of the theory are found to be in accord with the previous observations of Borrmann and Campbell. The theory further predicts that the peaks in the reflected and transmitted beams would not be coincident and this requires further verification.

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