X-RAY ANTI-REFLECTIONS IN CRYSTALS

Part II. Calculation of the Integrated Reflection and Integrated Anti-Reflection for an Internal Reflection

BY G. N. RAMACHANDRAN, F.A.SC.
(*Department of Physics, University of Madras, Guindy, Madras-25*)

Received December 21, 1953

1. INTRODUCTION

THE influence of the state of perfection of a crystal on the integrated reflection was considered by Hirsch and the author (1950) for the case of a surface reflection. The present paper deals with a similar study for an internal reflection, *i.e.*, when both the incident and reflected beams pass through the thickness of the crystal. The basic theory for an internal reflection is contained in the dynamical theory of Ewald (1916), which has been amplified and put in a more tractable form recently by Zachariasen (1945) and Laue (1949). Using these, the interesting observations of Campbell (1951) on the occurrence of sharp maxima in the transmitted beam have been explained by the author (1952 *a*, *b*) and independently by Hirsch (1952). This phenomenon has been termed "anti-reflection" by the author, and arises essentially from a decrease in the absorption coefficient near a reflection maximum, as has been pointed out by Laue (1949) and shown to be quantitatively true by Zachariasen (1952).

In the present paper we shall consider the variations of the reflected and transmitted intensities with various factors such as absorption coefficient, structure factor, asymmetry and thickness of the crystal. It is found that Laue's equations, which formed the basis of the previous paper of the author (Ramachandran and Kartha, 1952 *b*, hereafter referred to as Part I), are not accurate enough as they had been obtained by putting in certain approximations in the very beginning. Consequently, more complete expressions are worked out here and the approximations for special cases are obtained later.

The notation of Part I will be used in this paper, and reference may be made to Section 3 of that paper for the explanation of the symbols. Additional symbols used are collected together in the next section for ready reference.

2. NOTATION

P $= \frac{\mu D}{2}\left(\frac{1}{\gamma_0} + \frac{1}{\gamma_h}\right)$, product of the absorption coefficient and the mean path through the crystal of the reflected and transmitted beams.

G $= g/a$, parameter depending on the relative values of absorption coefficient and structure factor.

a $= (1 - b)/(1 + b)$, asymmetry factor.

X $= [(y^2 - a^2G^2 + 1 - k^2) + i(k + ayG)]^{\frac{1}{2}}$

j $= (a^2 + k^2/G^2)^{\frac{1}{2}}$

ϕ $= \tan^{-1} aG/k$.

R_y $= \int_{-\infty}^{+\infty} R\,dy$, integrated reflection in y-units.

T_y $= \int_{-\infty}^{+\infty} (T - e^{-\mu D/\gamma_0})\,dy$, integrated transmission in y-units.

3. EXACT EXPRESSIONS FOR R AND T IN THE CASE OF AN INTERNAL REFLECTION

We have the following equations from Laue's paper:

$$D_{01} = \frac{e^{-\nu}}{2\cosh\nu} D_0^{(a)} \quad ; \quad D_{02} = \frac{e^{+\nu}}{2\cosh\nu} D_0^{(a)} \tag{1}$$

$$D_{h1} = \frac{-\sqrt{b}}{2\cosh\nu}\left[\frac{\chi_{\bar{h}}}{\chi_h}\right]^{\frac{1}{2}} D_0^{(a)} \quad ; \quad D_{h2} = \frac{+\sqrt{b}}{2\cosh\nu}\left[\frac{\chi_{\bar{h}}}{\chi_h}\right]^{\frac{1}{2}} D_0^{(a)}, \tag{2}$$

where $\sinh\nu = \beta_h \sqrt{b}/2C\,[\chi_h\chi_{\bar{h}}]^{\frac{1}{2}}$ (3)

Introducing the variable

$$\epsilon_h = b\beta_h/2 = b\alpha_h + \chi_0(1 - b)/2, \tag{4}$$

we have

$$\sinh\nu = \epsilon_h/C\sqrt{b}\,[\chi_h\,\chi_{\bar{h}}]^{\frac{1}{2}} \tag{5}$$

The boundary conditions give the equations*

$$D_{01}\exp[-2\pi i(\mathbf{R}_{01}\cdot\mathbf{z})D] + D_{02}\exp[-2\pi i(\mathbf{R}_{02}\cdot\mathbf{z})D] = D_0^{(d)}\exp[-2\pi i(\mathbf{R}_0^{(d)}\cdot\mathbf{z})D] \tag{6 a}$$

$$D_{h1}\exp[-2\pi i(\mathbf{R}_{h1}\cdot\mathbf{z})D] + D_{h2}\exp[-2\pi i(\mathbf{R}_{h2}\cdot\mathbf{z})D] = D_h^{(d)}\exp[-2\pi i(\mathbf{R}_h^{(d)}\cdot\mathbf{z})D] \tag{6 b}$$

* The corresponding Eq. (6) in Part I contains a small obvious error, which, however, does not affect the final results.

Here

$$\mathbf{R}_{h1,2} = \mathbf{R}_{01,2} + \mathbf{b}_h$$

and

$$\mathbf{R}_{01,2} = \mathbf{R}_0^{(a)} - k\delta_{1,2}\mathbf{z} \tag{7}$$

where

$$\delta_{1,2} = \frac{1}{2\gamma_0}(\epsilon_h - \chi_0) \pm \frac{1}{2\gamma_0}(\epsilon_h^2 + bC^2\chi_h\chi_{\bar{h}})^{\frac{1}{2}}, \tag{8}$$

the positive sign referring to field No. 1 and the negative sign to field No. 2. Thus,

$$|D_h^{(d)}|^2 = |D_{h1}\exp(2\pi ik\delta_1 D) - D_{h2}\exp(2\pi ik\delta_2 D)|^2.$$

Writing

$$\sigma_{1,2} = 4\pi k \,\mathrm{Im}(\delta_{1,2}) \text{ and } \Delta_{1,2} = -4\pi k \,\mathrm{Re}(\delta_{1,2}), \tag{9}$$

where the symbols Im and Re stand for the imaginary and real parts of δ, we have

$$R = \frac{1}{b}\left|\frac{D_h^{(d)}}{D_0^{(a)}}\right|^2 = \frac{\exp[-\frac{1}{2}(\sigma_1+\sigma_2)D]}{2|\cosh\nu|^2}\left|\frac{\chi_{\bar{h}}}{\chi_h}\right| \times[\cosh\tfrac{1}{2}(\sigma_1-\sigma_2)D - \cos\tfrac{1}{2}(\Delta_1-\Delta_2)D] \tag{10}$$

From Eqn. (6 *a*), the corresponding expression for the transmission T can readily be shown to be

$$T = \left|\frac{D_0^{(d)}}{D_0^{(a)}}\right|^2 = \frac{\exp[-\frac{1}{2}(\sigma_1+\sigma_2)D]}{2|\cosh\nu|^2}[\cosh\{\tfrac{1}{2}(\sigma_1-\sigma_2)D + 2\nu_r\} + \cos\{\tfrac{1}{2}(\Delta_1-\Delta_2)D + 2\nu_i\}] \tag{11}$$

Equations (10) and (11) do not use the approximation adopted by Laue, namely, that the imaginary part of ν is small, and that $|\cosh\nu|^2 = \cosh^2\nu_r$.

4. Formulae for Centro-Symmetric Crystals

When a crystal possesses a centre of symmetry, the symmetry operation of inversion requires that $\chi_h = \chi_{\bar{h}}$.

Under these conditions,

$$\chi_h\chi_{\bar{h}} = \chi_h^2 \text{ and } |\chi_h/\chi_{\bar{h}}| = 1.$$

Thus,

$$\sinh\nu = \epsilon_h/C\sqrt{b}\chi_h \tag{12}$$

and

$$\delta_{1,2} = \frac{1}{2\gamma_0}(\epsilon_h - \chi_0) \pm \frac{1}{2\gamma_0}(\epsilon_h^2 + bC^2\chi_h^2)^{\frac{1}{2}}. \tag{13}$$

Defining

$$\left.\begin{aligned} y &= \epsilon_{hr}/C \mid \chi_{hr} \mid b^{\frac{1}{2}} \\ g &= \epsilon_{hi}/C \mid \chi_{hr} \mid b^{\frac{1}{2}} \\ k &= \chi_{hi}/\chi_{hr} \end{aligned}\right\} \quad (14)$$

we have

$$\sinh v = (y + ig)/(1 + ik) \quad (15)$$

One thus obtains the following expressions for the various quantities occurring in Eqs. (10) and (11) in terms of the parameters y, g, k, which are the same as those used by Zachariasen (1945).

$$\cosh^2 v = [(y + ig)^2 + (1 - k^2 + 2ik)]/(1 - k^2 + 2ik)$$

$$| \cosh^2 v | = [(y^2 - g^2 + 1 - k^2)^2 + 4(k + yg)^2]^{\frac{1}{2}}/(1 + k^2) \quad (16)$$

$$\tfrac{1}{2}(\sigma_1 + \sigma_2) = -2\pi k \chi_{0i}(1 + b)/2\gamma_0 = \mu(1 + b)/2\gamma_0$$

$$\tfrac{1}{2}(\sigma_1 - \sigma_2) = [2\pi k C\chi_{hr}/\sqrt{\gamma_h\gamma_0}]\ \mathrm{Im}\,[(y^2 - g^2 + 1 - k^2) + 2i(k + yg)]^{\frac{1}{2}}$$

$$\tfrac{1}{2}(\Delta_1 - \Delta_2) = [2\pi k C\chi_{hr}/\sqrt{\gamma_h\gamma_0}]\ \mathrm{Re}\,[(y^2 - g^2 + 1 - k^2) + 2i(k + yg)]^{\frac{1}{2}}$$

Defining a new parameter

$$G = \tfrac{1}{2}\chi_{0i}(1 + b)/C\sqrt{b} \mid \chi_{hr} \mid = g/a, \quad (17)$$

where a is the asymmetry factor

$$a = (1 - b)/(1 + b) \quad (18)$$

we have

$$2\pi k C\chi_{hr}/\sqrt{b} = \frac{2\pi k \chi_{0i}}{G}\,\frac{(1 + b)}{2\gamma_0} = -\frac{\mu}{G}\,\frac{(1 + b)}{2\gamma_0}$$

Writing

$$\mu D(1 + b)/2\gamma_0 = \frac{\mu D}{2}\left(\frac{1}{\gamma_0} + \frac{1}{\gamma_h}\right) = P, \quad (19)$$

which is only an obvious generalisation of the definition of P in Part I, we have

$$R = \frac{e^{-P}(1 + k^2)}{2|X|^2}\left[\cosh\left(\frac{P}{G}\,\mathrm{Im}\,X\right) - \cos\left(\frac{P}{G}\,\mathrm{Re}\,X\right)\right], \quad (20)$$

$$T = \frac{e^{-P}(1 + k^2)}{2|X|^2}\left[\cosh\left(\frac{P}{G}\,\mathrm{Im}\,X - 2v_r\right) + \cos\left(\frac{P}{G}\,\mathrm{Re}\,X - 2v_i\right)\right], \quad (21)$$

where

$$X = [(y^2 - a^2G^2 + 1 - k^2) + 2i(k + ayG)]^{\frac{1}{2}} \quad (22)$$

On making the approximations $k \ll 1$ and $v_i \ll 1$, one obtains Eqns. (8) and (9) of Part I, which were deduced directly from Laue's paper.

5. Expressions for Integrated Reflection

All the quantities occurring in Eqns. (20) and (21) are constant parameters for a particular reflection of a crystal, except y, which is proportional to the angular deviation from the exact Bragg setting. Thus, a graph of R (or T) against y represents the Bragg reflection (or anti-reflection) curve. Except in special experiments, employing high resolution, one is interested in general, not in the shape or breadth of this curve, but in the " integrated " quantity, which is the area enclosed between this curve and the axis of abscissæ. The integrated reflection (or anti-reflection) in y-units, *viz.*, $\int_{-\infty}^{+\infty} \mathrm{R}dy$ is actually proportional to the integrated reflection, as usually understood, *viz.*, $\int_{-\infty}^{+\infty} \mathrm{R}d(\theta - \theta_{\mathrm{B}})$, the relation between the two being given by

$$\int \mathrm{R}d(\theta - \theta_{\mathrm{B}}) = \frac{\mathrm{C}\,|\,\chi_h\,|}{\sqrt{b}\sin 2\theta_{\mathrm{B}}} \int \mathrm{R}dy \tag{23}$$

Consequently, we shall only use the former to represent the integrated reflection, and denote it by the symbol R_y (or T_y as the case may be).

The integration may be carried out analytically in a few cases and we shall consider these below:

(*a*) For a symmetrical reflection, $a = 0$, and if k is small, so that $k^2 \ll 1$, then we have

$$\mathrm{X} \simeq [(y^2+1) + 2ik]^{\frac{1}{2}} = (y^2+1)^{\frac{1}{2}} + ik/(y^2+1)^{\frac{1}{2}}$$

and

$$|\,\mathrm{X}\,|^2 = (y^2+1)$$

Thus,

$$\mathrm{R}_y = \frac{e^{-\mathrm{P}}}{2} \int_{-\infty}^{+\infty} \frac{1}{(y^2+1)} \left[\cosh \frac{\mathrm{P}k}{\mathrm{G}\sqrt{y^2+1}} - \cos \frac{\mathrm{P}\sqrt{y^2+1}}{\mathrm{G}}\right] dy$$

which may be put in the form:

$$\mathrm{R}_y = \frac{e^{-\mathrm{P}}}{2} \left[\int_{-\pi/2}^{\pi/2} \cosh\left(\frac{\mathrm{P}k\cos\theta}{\mathrm{G}}\right) d\theta - \int_{-\infty}^{+\infty} \frac{\cos[\mathrm{P}(\cosh t)/\mathrm{G}]}{\cosh t}\, dt\right].$$

Both the integrals can be expressed in terms of standard Bessel Functions, so that we have

$$R_y = \frac{\pi}{2} e^{-P} \left[I_0 (kP/G) - 1 + \int_0^{P/G} J_0 (x)\, dx \right] \tag{24}$$

$$= \frac{\pi}{2} e^{-P} \left[I_0 (kP/G) - 1 + 2 \sum_{n=0}^{\infty} J_{2n+1} (P/G) \right] \tag{25}$$

(*b*) Another special case in which the expression (20) can be integrated in analytical terms is when $a \neq 0$, but aG is small, so that $a^2G^2 \ll 1$, with $k^2 \ll 1$ as previously.

Under these conditions, we have

$$X \simeq [(y^2 + 1) + 2i (k + aGy)]^{\frac{1}{2}}$$
$$= (y^2 + 1)^{\frac{1}{2}} + i (k + aGy)/(y^2 + 1)^{\frac{1}{2}}$$

and

$$|X|^2 = y^2 + 1, \text{ as before.}$$

The integral R_y can now be put in the form

$$R_y = \frac{e^{-P}}{2} \left[\int_{-\pi/2}^{\pi/2} \cosh [jP \cos (\theta - \phi)]\, d\theta - \int_{-\infty}^{+\infty} \frac{\cos [(P/G) \cosh t]}{\cosh t}\, dt \right]$$

where

$$j^2 = a^2 + (k/G)^2 \text{ and } \tan \phi = aG/k. \tag{26}$$

Thus,

$$R_y = \frac{\pi}{2} e^{-P} \left[I_0 (jP) - 1 + \int_0^{P/G} J_0 (x)\, dx \right]. \tag{27}$$

Obviously this reduces to Eqn. (24) of case (*a*) when $a = 0$.

(*c*) Another special case in which the expression (20) for R can be integrated is when $a \neq 0$ and $G^2 \gg 1$. Under these conditions, one has

$$X \simeq [y^2 - a^2G^2 + 2iayG]^{\frac{1}{2}} = [y + iaG]$$

and

$$|X|^2 = y^2 + a^2G^2.$$

Thus,

$$R_y = \frac{e^{-P} (1 + k^2)}{2} \int_{-\infty}^{+\infty} [\cosh aP - \cos (Py/G)]/(y^2 + a^2G^2)\, dy.$$

Now,

$$\int_{-\infty}^{+\infty} dy/(y^2 + a^2G^2) = \pi/aG$$

and

$$\int_{-\infty}^{+\infty} \cos (Py/G)\, dy/(y^2 + a^2G^2) = \pi e^{-|aP|}/|aG|$$

(Madelung, 1950), so that

$$R_y = \frac{\pi(1 + k^2)}{2|aG|} e^{-P} (\cosh aP - e^{-|aP|})$$

$$= \frac{\pi}{2G} (1 + k^2) e^{-P} \frac{\sinh aP}{a} \tag{28}$$

As will be shown below, this is identical with the corresponding integrated reflection in y-units for a mosaic crystal.

6. Expressions for Integrated Anti-Reflection

The integrated anti-reflection in y-units will be denoted by the symbol T_y and is defined as

$$T_y = \int_{-\infty}^{+\infty} (T - e^{-\mu D/\gamma_0})\, dy. \tag{29}$$

Here, $\exp(-\mu D/\gamma_0)$ is the fraction of the incident intensity which is normally transmitted in the absence of Bragg reflection, and the integrated anti-reflection is the integral over various settings of the excess (or defect) of the actual transmission over this background.

(*a*) *Symmetrical Case.*—Here, $a = 0$, which corresponds to case (*a*) of the previous section and the integration may be carried out analytically. Thus, taking $k^2 \ll 1$ as before, one has

$$T = \frac{e^{-P}}{2(1 + y^2)} \left[\cosh\left(\frac{P}{G} \operatorname{Im} X - 2v_r\right) + \cos\left(\frac{P}{G} \operatorname{Re} X - 2v_i\right)\right]. \tag{30}$$

Now,

$$\sinh v = y/(1 + ik) = y - iky, \tag{31}$$

so that, within the limits of approximation adopted here,

$$\left.\begin{aligned} \sinh v_r &= y, & \sin v_i &= -ky/(y^2 + 1)^{\frac{1}{2}} \\ \cosh 2v_r &= 1 + 2y^2, & \cos 2v_i &= 1 \end{aligned}\right\} \tag{32}$$

Also, in the symmetrical case,

$$e^{-\mu D/\gamma_0} = e^{-P},$$

On expanding the cosh and cos functions within the square brackets in (30) into products of similar functions, all the odd functions of y drop out of the integral, since the range of integration is from $-\infty$ to $+\infty$, so that we have

$$T_y = e^{-P} \int_{-\infty}^{+\infty} \left[\frac{\cosh 2v_r}{2(1+y^2)} \cosh (Pk/G\sqrt{y^2+1}) + \frac{\cos 2v_i}{2(1+y^2)} \cos \frac{P\sqrt{y^2+1}}{G} - 1 \right] dy$$

Substituting from (32), and rearranging the terms, one obtains

$$T_y = e^{-P} \int_{-\infty}^{+\infty} [\cosh (Pk/G\sqrt{y^2+1}) - 1]\, dy - R_y \tag{33}$$

Making the substitution $y = \tan \theta$, the integral in (33) becomes

$$\int_{-\pi/2}^{+\pi/2} \frac{1}{\cos^2 \theta} \left[\cosh \left(\frac{Pk}{G} \cos \theta \right) - 1 \right] d\theta$$

which can be shown to be equal to

$$\pi \int_0^{Pk/G} dx' \int_0^{x'} I_0(x)\, dx \tag{34 a}$$

or

$$= \pi (Pk/G) \int_0^{Pk/G} I_1(x)/x\, dx \tag{34 b}$$

Here $I_0(x)$ and $I_1(x)$ are the Bessel functions of imaginary argument of order zero and one respectively [$J_0(ix)$ and $J_1(ix)$]. The proof is given in Appendix I. Thus, finally,

$$T_y = \pi e^{-P} \int_0^{Pk/G} dx' \int_0^{x'} I_0(x)\, dx - R_y \tag{35}$$

$$= \pi e^{-P} \left[\int_0^{Pk/G} dx' \int_0^{x'} I_0(x)\, dx - \tfrac{1}{2} I_0(jP) + 1 - \int_0^{P/G} J_0(x)\, dx \right] \tag{36}$$

(*b*) *Asymmetrical Case, Small Absorption.*—Taking as in §5 (*b*) that $a^2G^2 \ll 1$ and $k^2 \ll 1$, we now have,

$$\sinh v = (y + iaGy)/(1 + ik) = y + i(aG - ky) \tag{37}$$

Thus,

$$\left.\begin{array}{ll} \sinh v_r = y, & \sin v_i = (aG - ky)/\sqrt{y^2+1} \\ \cosh 2v_r = 1 + 2y^2, & \cos 2v_i = 1 \end{array}\right\} \tag{38}$$

to the same degree of approximation as in the last sub-section.

Also,

$$\text{Im X} = (k + a\text{G}y)/(y^2 + 1)^{\frac{1}{2}}$$

and

$$\text{Re X} = (y^2 + 1)^{\frac{1}{2}}.$$

Thus, from Eqn. (30),

$$\text{T} = \frac{e^{-\text{P}}}{2\,(1+y^2)} \left[\cosh \left\{\frac{\text{P}\,(k+a\text{G}y)}{\text{G}\,(y^2+1)^{\frac{1}{2}}} - 2v_r\right\} + \cos \left\{\frac{\text{P}}{\text{G}}\,(y^2 + 1)^{\frac{1}{2}} - 2v_i\right\}\right]. \tag{39}$$

The background intensity exp $-\mu\text{D}/\gamma_0$ can be put in the form exp $[-\text{P}\,(1 + a)]$ and we therefore have, from Eq. (29), leaving out the odd terms:

$$\text{T}_y = e^{-\text{P}} \int_{-\infty}^{+\infty} \left[\frac{1 + 2y^2}{2\,(1 + y^2)} \cosh \frac{\text{P}\,(k + a\text{G}y)}{\text{G}\,(y^2 + 1)^{\frac{1}{2}}} - e^{-a\text{P}} + \frac{1}{2\,(1 + y^2)} \cos \frac{\text{P}}{\text{G}}\,(y^2 + 1)^{\frac{1}{2}} + \frac{a\text{G}}{2\,(1 + y^2)^{3/2}} \sin \frac{\text{P}}{\text{G}}\,(y^2 + 1)^{\frac{1}{2}}\right] dy \tag{40}$$

With the help of suitable transformations, this can be put in the form:

$$\text{T}_y = e^{-\text{P}} \int_{-\pi/2}^{\pi/2} \frac{1}{\cos^2\theta}\,[\cosh\,(j\text{P}\cos\overline{\theta - \phi}) - \sin\theta\sinh\,(j\text{P}\cos\overline{\theta - \phi}) - e^{-a\text{P}}]\,d\theta - \frac{e^{-\text{P}}}{2}\int_{-\pi/2}^{\pi/2}\cosh\,(j\text{P}\cos\overline{\theta - \phi})\,d\theta + \frac{e^{-\text{P}}}{2}\int_{-\infty}^{+\infty}\frac{\cos\left(\frac{\text{P}}{\text{G}}\cosh t\right)}{\cosh t}\,dt + \frac{e^{-\text{P}}}{2}\,a\text{G}\int_{-\infty}^{+\infty}\frac{\sin\left(\frac{\text{P}}{\text{G}}\cosh t\right)}{\cosh^2 t}\,dt, \tag{41}$$

where $j = (a^2 + k^2\text{G}^2)^{\frac{1}{2}}$ and $\tan\phi = a\text{G}/k$ (see Appendix II). Making use of the expression for R_y from Eqn. (26), we find that the second and third terms together are exactly $= -\,\text{R}_y$, so that

$$T_y + R_y = e^{-P} \int_{-\pi/2}^{\pi/2} \frac{1}{\cos^2\theta} [\cosh(jP\cos\overline{\theta-\phi}) - \sin\theta\sinh(jP\cos\overline{\theta-\phi}) - e^{-aP}]\,d\theta + \frac{e^{-P}}{2} aG \int_{-\infty}^{+\infty} \sin\left(\frac{P}{G}\cosh t\right)\Big/\cosh^2 t\,dt \qquad (42)$$

Both of these can be integrated (Appendix II) and finally we have

$$T_y + R_y = \pi e^{-P} \Big[jP \int_0^{jP} I_1(x)/x\,dx + \tan\phi\ (\text{integrals involving } jP \text{ and } \phi) + aG \int_0^{P/G} dx' \int_0^{x'} J_0(x)\,dx \Big] \qquad (43)$$

It is readily seen that, when $a = 0$, *i.e.*, $\phi = 0$, this reduces to Eqn. (35) for the symmetrical case.

7. VARIATION OF INTEGRATED REFLECTION AND ANTI-REFLECTION WITH VARIOUS FACTORS

(*a*) *Integrated Reflection.*—The relevant formulæ are given by Eqns. (24), (25), (27) and (28). Firstly, for ordinary reflections, which are not too weak, the quantity G is usually small, of the order of 0·1 or less, so that P/G is large, for ordinary thicknesses of the order of a millimetre. Consequently, the integral is nearly equal to unity and Eqns. (27) and (36) reduce to

$$R_y = \frac{\pi}{2} e^{-P} I_0(jP) \qquad (44)$$

$$T_y = \pi e^{-P} \Big[jP \int_0^{jP} I_1(x)/x\,dx - \tfrac{1}{2} I_0(jP) \Big] \qquad (45)$$

Consequently, for moderate and large values of P, the integrated reflection varies as $e^{-P} I_0(jP)$. The effect of the terms left out of Eqn. (24) is to produce small fluctuations in this curve close to the origin. In fact, Eqn. (44) does not hold for small values of $P \to 0$, and the limiting value is not $\pi/2$, as would be given by this equation, but is equal to zero. This follows from the more accurate Eqn. (24), from which

$$\underset{P\to 0}{\text{Lt}}\, R_y = \frac{\pi}{2} \Big[1 - 1 + 2 \underset{P\to 0}{\text{Lt}}\, J_1(P/G) \Big], \quad (e^P \to 1)$$
$$= \underset{P\to 0}{\text{Lt}}\, \pi P/G = 0.$$

This is as it should be, since a crystal of zero thickness gives no reflection.

For small P, we have

$$R_y = \frac{\pi}{2G} Pe^{-P}, \tag{46}$$

which is exactly the same as that for a mosaic crystal of small thickness. In fact, if G is large, this equality of the integrated reflections of a perfect and a mosaic crystal holds over a much wider range. Eqn. (28) for a perfect crystal under these conditions is identical with the formula for a mosaic crystal (derived in Appendix III).

A large value of G signifies either that the crystal has a large absorption coefficient or that the structure amplitude of the reflection concerned is small. For a weak reflection, G is large even with medium absorption. In such a case, the formula for the integrated reflection of a perfect crystal is to be expected to be the same as that of a mosaic crystal. The reflected beam will not be allowed to build up by means of multiple reflections, owing to the heavy absorption, the beam being extinguished by absorption before the reinforcement by multiple reflections becomes effective. The mutual interaction of the incident and reflected beams throughout the bulk of the crystal, which is the essential consideration in the dynamical theory, thus ceases to be important, and it is therefore natural that the result of the more detailed dynamical theory agrees with that of the simple " kinematical " theory for a mosaic crystal.

For the same reason, even when G is not large, the result of the two theories agree for small values of P [(Eqn. (46)], *i.e.*, for small thicknesses.

(*b*) *Integrated Transmission.*—The most interesting result is that the integrated transmission may be either positive or negative, according to the conditions of the experiment. For small thicknesses, it is negative, as is to be expected from the shape of the reflection curve reported in Part I. As the thickness increases, there comes a stage, when the reflection curve contains both a dip below and a peak above the background, and the *integrated* transmission is actually zero. For larger thicknesses than this, the integrated transmission is positive.

If the incident beam is not extremely well collimated (with an angular divergence less than 1″ of arc), the variations observed in the transmitted beam would not give the true changes in intensity predicted by theory. However, a strict comparison between theory and experiment is possible by measuring the *integrated* transmission using a much wider beam for study. The formulæ in the present paper were mainly developed for this purpose and further experiments are in progress. It may be mentioned that the formula (44) for the integrated reflection of an "internal" reflection has already been verified by Padmanabhan (1953).

8. SUMMARY

Making use of the theory developed in Part I, the integrated values of the reflected and the anti-reflected intensity have been obtained analytically for an internal reflection of a perfect crystal. Three special cases are considered, namely a symmetrical reflection, an asymmetrical reflection and also when absorption is very heavy. It is found that when absorption is large, the formula for integrated reflection reduces to that for a mosaic crystal, which may be physically explained by the fact that multiple reflections are not allowed to play a prominent part owing to the beam being quickly attenuated by absorption.

REFERENCES

1. Campbell, H. N. .. *J. Appl. Phys.*, 1951, **22**, 1139.
2. Ewald, P. B. .. *Ann. d. Phys.*, 1916, **49**, 1, 117.
3. Hirsch, P. B. and Ramachandran, G. N. *Acta Cryst.*, 1950, **3**, 187.
4. Hirsch, P. B. .. *Ibid.*, 1952, **5**, 176.
5. Laue, von M. .. *Ibid.*, 1949, **2**, 106.
6. Madelung, E. .. "*Die Mathematischen Hilfsmittel des Physikers*," Springer, Berlin, 1950, 47.
7. Padmanabhan, V. M. .. *J. Ind. Inst. Sci.*, 1953, **35**, 1.
8. Ramachandran, G. N. .. *J. Appl. Phys.*, 1952 *a*, **23**, 500.
9. ——— and Kartha, G. .. *Proc. Ind. Acad. Sci.*, 1952 *b*, **35A**, 145.
10. Watson, G. N. .. *Bessel Functions*, Cambridge, 1944, 79.
11. Zachariasen, W. H. .. *Theory of X-Ray Diffraction in Crystals*, Wiley, New York, 1945.
12. ——— .. *Proc. Nat. Acad. Sci.*, U.S.A., 1952, **38**, 378.

APPENDIX I

Proof of Results (34 *a*) and (34 *b*)

The integral to be evaluated is

$$\int_{-\pi/2}^{\pi/2} \frac{1}{\cos^2\theta}\,[\cosh(q\cos\theta) - 1]\,d\theta, \tag{47}$$

where $q = j\mathrm{P} = \mathrm{P}k/\mathrm{G}$.

From the standard expressions for the Bessel function $\mathrm{I}_0(x)$, we have

$$\pi\,\mathrm{I}_0(x) = \int_{-\pi/2}^{\pi/2} \cosh(x\cos\theta)\,d\theta \tag{48}$$

Integrating this

$$\pi\int_0^{x'} \mathrm{I}_0(x)\,dx = \int_{-\pi/2}^{\pi/2} \left[\frac{\sinh(x\cos\theta)}{\cos\theta}\right]_0^{x'} d\theta.$$

$$= \int_{-\pi/2}^{\pi/2} \frac{\sinh(x'\cos\theta)}{\cos\theta}\,d\theta \tag{49}$$

Integrating again,

$$\pi\int_0^{q} dx' \int_0^{x'} \mathrm{I}_0(x)\,dx = \int_{-\pi/2}^{\pi/2} \left[\frac{\cosh(x'\cos\theta)}{\cos^2\theta}\right]_0^{q} d\theta$$

$$= \int_{-\pi/2}^{\pi/2} \frac{1}{\cos^2\theta}\,[\cosh(q\cos\theta) - 1]\,d\theta. \tag{50}$$

The right-hand side is identical with the expression (47), which proves the result (34 *a*).

We may also proceed in another manner by first integrating (47) by parts. We thus have

$$(47) = \int_{-\pi/2}^{\pi/2} \{\cosh(q\cos\theta) - 1\}\,d(\tan\theta)$$

$$= \Big[\tan\theta\,\{\cosh(q\cos\theta) - 1\}\Big]_{-\pi/2}^{\pi/2} + \int_{-\pi/2}^{\pi/2} \frac{1}{\cos\theta}\,q\sin^2\theta\sinh(q\cos\theta)\,d\theta. \tag{51}$$

The first term of (51) vanishes and since (Watson, 1944)

$$\pi\, I_1(x) = x \int_{-\pi/2}^{\pi/2} \sin^2\theta \cosh(x\cos\theta)\, d\theta,$$

the second term is equal to

$$\pi\, q \int_0^q I_1(x)/x\, dx, \tag{52}$$

which is the result (34 *b*).

APPENDIX II

Simplification of the Integrals in Eqn. (42)

The integral to be evaluated is

$$\int_{-\pi/2}^{\pi/2} \frac{1}{\cos^2\theta} [\cosh(jP\cos\overline{\theta-\phi}) - \sin\theta \sinh(jP\cos\overline{\theta-\phi}) - e^{-aP}]\, d\theta \tag{53}$$

where $j\sin\phi = a$. This may be written in the form

$$\int_{-\frac{\pi}{2}-\phi}^{\frac{\pi}{2}-\phi} \sec^2(\theta+\phi)\, [\cosh(jP\cos\theta) - \sin(\theta+\phi)\sinh(jP\cos\theta) - e^{-aP}]\, d\theta \tag{54}$$

Integrating by parts as in the previous Appendix I, we obtain

$$\Big[\tan(\theta+\phi)\cosh(jP\cos\theta) - \sec(\theta+\phi)\sinh(jP\cos\theta) - e^{-aP}\Big]_{-\frac{\pi}{2}-\phi}^{\frac{\pi}{2}-\phi}$$

$$+ \int_{-\frac{\pi}{2}-\phi}^{\frac{\pi}{2}-\phi} \tan(\theta+\phi)\, jP\sin\theta \sinh(jP\cos\theta)\, d\theta$$

$$- \int_{-\frac{\pi}{2}-\phi}^{\frac{\pi}{2}-\phi} \sec(\theta+\phi)\, jP\sin\theta\cosh(jP\cos\theta)\, d\theta.$$

The first term is again equal to zero, and making the substitutions

$$\tan(\theta+\phi) = \tan\theta + \tan\phi + \tan\theta\tan\phi\tan(\theta+\phi) \tag{56}$$

and $$\sec(\theta+\phi) = \sec\theta\sec\phi + \tan\theta\tan\phi\sec(\theta+\phi) \tag{57}$$

in (55) and putting $jP = q$, we get the integral (53) as

$$\int_{-\frac{\pi}{2}-\phi}^{\frac{\pi}{2}-\phi} (q/\cos\theta)\sin^2\theta \sinh(q\cos\theta)d\theta$$
$$+ \int q\tan\phi \sin\theta \sinh(q\cos\theta)\,d\theta$$
$$+ \int q\tan\phi (\sin^2\theta/\cos\theta)\tan(\theta+\phi)\sinh(q\cos\theta)\,d\theta$$
$$- \int q\sec\phi \tan\theta \cosh(q\cos\theta)\,d\theta$$
$$- \int q\tan\phi(\sin^2\theta/\cos\theta)\sec(\theta+\phi)\cosh(q\cos\theta)\,d\theta \qquad (58)$$

The second and the fourth terms vanish, and the first term can be shown to be equal to (52), so that we finally obtain the integral (53) in the form

$$\pi jP \int_0^{jP} I_1(x)/x\,dx$$
$$+ \tan\phi \left[\int_{-\frac{\pi}{2}-\phi}^{\frac{\pi}{2}-\phi} jP(\sin^2\theta/\cos\theta)\tan(\theta+\phi)\sinh(jP\cos\theta)\,d\theta \right.$$
$$\left. - \int_{-\frac{\pi}{2}-\phi}^{\frac{\pi}{2}-\phi} jP(\sin^2\theta/\cos\theta)\sec(\theta+\phi)\cosh(jP\cos\theta)\,d\theta \right] \qquad (59)$$

APPENDIX III

Derivation of R_y for an Internal Reflection given by a Mosaic Crystal

If Q stands for the well-known expression

$$Q = \frac{C}{\sin 2\theta_B}\frac{e^4}{m^2c^4}\lambda^3F^2N^2 \quad (C = 1 \text{ or } \cos^2\theta) \qquad (60)$$

and D is the thickness of the crystal slab, then the integrated reflection for the whole crystal is

$$\int_0^D \frac{Q}{\gamma_0}\exp\left[-\frac{\mu x}{\gamma_0} - \frac{\mu(D-x)}{\gamma_h}\right]dx$$
$$= \frac{Q}{\mu(1-\gamma_0/\gamma_h)}\exp\left[-\frac{\mu D}{2}\left(\frac{1}{\gamma_0}+\frac{1}{\gamma_h}\right)\right]\cdot 2\sinh\left[\frac{\mu D}{2}\left(\frac{1}{\gamma_0}-\frac{1}{\gamma_h}\right)\right] \qquad (61)$$

Putting $\frac{\mu D}{2}\left(\frac{1}{\gamma_0}+\frac{1}{\gamma_h}\right)=P$ and $(1-b)/(1+b)=a$ (the asymmetry factor), this becomes

$$=\frac{2Q}{\mu(1+b)}e^{-P}\frac{\sinh aP}{a} \tag{62}$$

Converting into the y-scale, we have

$$R_y\,(\text{mosaic})=\frac{\pi}{2G}e^{-P}\frac{\sinh aP}{a} \tag{63}$$