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THE REFLECTION OF X-RAYS BY CRYSTALS AS A PROBLEM IN THE REFLECTION OF RADIATION BY PARALLEL PLANES

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ABSTRACT

It is pointed out that the previous solutions of the problem of the reflection of radiation from parallel planes by Lamson and Gronwall are physically incorrect since the intensities, not the amplitudes, of contributions from individual planes, have been added. It is shown that a mathematical method due to Darwin leads to a solution identical mathematically with those of Lamson and Gronwall. Using this result, the intensity of reflection is evaluated for certain ranges of the constants directly related to the reflected and transmitted amplitudes due to a single plane.

THE problem of the reflection and transmission of radiation by a set of parallel, equidistant, reflecting planes has been treated by Darwin[1], Lamson[2], and recently, Gronwall[3]. The solution of this problem is at least of theoretical interest in the treatment of the intensity of reflection of x-rays by crystals, for if we adopt the Bragg picture of the reflection of x-rays by atomic planes, as contrasted with the space-lattice treatment of Laue, the reflection and transmission of a crystal sheet for an incident x-ray beam is essentially a problem of this type. The treatment of the problem of the reflection of x-rays by the methods used in the optics of isotropic media has been criticised by Ewald[4], but recently Bragg, Darwin and James[5], have pointed out that the methods used by Darwin give results almost identical with those of Ewald.

The treatments of the problem by Lamson and Gronwall, while excellent mathematically, are open to he fundamental objection that in computing the total reflection as a function of the amount reflected from each plane, the *intensities* from each plane have been added. Now in any practical case, and certainly in the crystalline reflection of x-rays, the

[1] Darwin, Phil. Mag. **27,** 675 (1914).
[2] Lamson, Phys. Rev. **17,** 624 (1921).
[3] Gronwall, Phys. Rev. **27,** 277 (1926).
[4] Ewald, Zeits. f. Physik **30,** 1 (1924); Ann d. Physik **54,** 519 (1918).
[5] Bragg, Darwin, and James, Phil. Mag. **1,** 897 (1926).

waves in question are coherent, and instead of their intensities, their *amplitudes* should be added. Nevertheless it can be shown that a large part of the mathematical work laid down by these authors is useful in the physically correct solution of the problem. The mathematical treatment of Gronwall is complete and elegant; he has obtained a solution intended to give the amount of radiation reflected from an incident beam of unit intensity by an infinite number of parallel planes, and also to give the amounts reflected and transmitted by a finite number of planes. The solutions for a finite number of planes are exceedingly complicated when expressed in terms of the constants of one plane and will not be considered here. The principal purpose of this paper is to attempt to give an acceptable physical meaning to the mathematical results of Gronwall for the reflection from an infinite number of parallel planes.

Let us consider the incidence of a monochromatic, parallel (an obvious idealisation), beam of x-rays of unit amplitude upon the face of a perfect crystal at the proper angle for reflection according to the Bragg law. We will neglect the influence of the index of refraction, also the polarisation and temperature corrections etc. According to the Bragg picture we can consider the atoms reflecting the x-rays to be arranged in planes. Let R_1 be the amplitude reflected by a single plane, and let T_1 be the amplitude of the wave emerging from the lower side of the plane, that is, the transmitted amplitude. Let R_n be the amplitude of the total wave reflected by n planes (as it emerges above the crystal face) considering all possible internal multiple reflections, and T_n be the amplitude of the total wave transmitted by n planes. Then following the method of Gronwall it is easily shown that the following equations hold[6].

$$R_{n+1}=R_n+T_n{}^2R_1/(1-R_1R_n) \tag{1}$$

$$T_{n+1}=T_nT_1/(1-R_1R_n) \tag{2}$$

These are second order difference equations, and if R is the amplitude of reflection from an infinite number of planes, Gronwall has shown[7] that they lead to the result.

[6] These equations may be obtained from Eqs. (8) and (7) of Gronwall's paper by making the substitutions $t=T_1$, $r=R_1$, $R_n'=R_n-R_1$. The introduction of R' terms in Gronwall's treatment is unnecessary.

[7] The radical in (3) comes in as the result of solving a quadratic equation, and Gronwall gives reasons for selecting the proper sign before the radical which are not valid for the case where amplitudes, and not intensities, are added. Nevertheless, an argument valid for the present treatment may be advanced which leads to the same selection of sign. Referring to Gronwall's paper, the quadratic to be solved is his Eq. (18). In carrying through the treatment in the notation of this article, we would let $\rho_n=1-R_1R_n$; then Gronwall's (18) becomes

$$\rho+T_1{}^2/\rho=\rho_1+T_1{}^2$$

$$R=(1/2R_1)(1-T_1^2+R_1^2-[(1+T_1^2-R_1^2)^2-4T_1^2]^{\frac{1}{2}}) \quad (3)$$

It is interesting to note that this same result was obtained with a slightly different method of approach by Darwin[8], though it is not explicitly stated in his paper in exactly this form. With Darwin let t_n be the amplitude of the total transmitted wave above the $(n+1)$st plane. Then t_0 is the amplitude of the incident beam. If r_n is the amplitude of the total reflected wave above the $(n+1)$st plane, then r_0 is that of the reflected beam from an infinite number of planes. As before let R_1 and T_1 be the amplitudes of the waves reflected and transmitted by a single plane. Then it follows that

$$r_n=R_1t_n+T_1r_{n+1} \quad (4)$$

$$t_{n+1}=T_1t_n+R_1r_{n+1} \quad (5)$$

If we eliminate r from these equations, we obtain

$$T_1(t_{n-1}+t_{n+1})=t_n(1+T_1^2-R_1^2) \quad (6)$$

Darwin now assumes a solution of the form

$$t_n=t_0x^n \quad (7)$$

Solving for x after insertion in (6) gives

$$2T_1x=1+T_1^2-R_1^2\pm[(1+T_1^2-R_1^2)^2-4T_1^2]^{\frac{1}{2}} \quad (8)$$

in which it is easily shown[9] that the negative sign alone gives a result of physical significance.

From (7) and Eqs. (4) and (5) we may also obtain

$$(r_0/t_0)=(1/2R_1)(2R_1^2+2T_1x-2T_1^2) \quad (9)$$

and if we substitute the correct value of x from (8)

$$r_0/t_0=(1/2R_1)(1-T_1^2+R_1^2-[(1+T_1^2-R_1^2)^2-4T_1^2]^{\frac{1}{2}}) \quad (10)$$

This is the result of Gronwall and Lamson if we consider t_0 as unity. The method of Darwin thus involves only first order difference equations, but Gronwall's method seems more readily adaptable to the study of reflec-

Now the product of the roots of this equation (solved for ρ), is T_1^2 and if they are unequal, one is greater and one less than T_1. But from our equation (2), the present ρ_n must be greater than T_1 or the amplitude of the transmitted beam would increase in the passage through the system. Thus the larger value of ρ is the physically significant one, as Gronwall concludes from other considerations.

[8] Darwin, Phil. Mag. **27**, 675, see p. 678 (1914).

[9] From the form of the quadratic from which (8) is obtained it follows that the product of the two roots given in (8) must be unity. If they are unequal, only the one less than unity can have physical significance by (7).

tion and transmission by a finite number of planes. Thus we see that three different methods of approach lead to the same solution, as expressed in (3).

If we consider the expression (3) for the amplitude of the reflected beam, we see that for a certain range of R_1 and T_1, namely $T_1 < 1 - R_1$. R will be imaginary. The physical significance of this is of course that there is a phase shift in reflection, and that

$$I = |R|^2 \tag{11}$$

where I is the intensity of the reflected beam.

Let us assume that the wave trains incident on, and reflected and transmitted by, a single plane, may be represented as follows.

$$y_i = \epsilon^{i\omega t} \tag{12}$$

$$y_r = b\epsilon^{i(\omega t + \delta)} \tag{13}$$

$$y_t = k\epsilon^{i\omega t} \tag{14}$$

Thus in (13) we assume a phase shift δ on reflection, but in (14) we neglect the shift in transmission. From these assumptions it follows that

$$R_1 = b\epsilon^{i\delta}, \quad T_1 = k \tag{15}$$

If we substitute these values in (3) and perform the operation indicated in (11) we should obtain an expression for the reflected intensity. Even with the simple assumptions (12), (13), (14), this expression becomes very complicated if the operations are carried out without auxiliary assumptions. We will first assume that δ is small so that $\epsilon^{i\delta} = 1 + i\delta$. We will also set $k = 1 - h$. Using these substitutions it follows, without neglecting any terms, that

$$\begin{aligned}[(1 - R_1^2 + T_1^2)^2 - 4T_1^2]^{\frac{1}{2}} = {} & [b^4 - 4b^2 + 2b^2h(2-h) \\ & + h^2(2-h)^2 - i\delta(8b^2 - 4b^4 - 4b^2h(2-h))]^{\frac{1}{2}}.\end{aligned} \tag{16}$$

If h and b are small, and terms of power higher than two may be neglected in comparison with $\pm(h^2 - b^2)$, this may be written

$$[(1 - R_1^2 + T_1^2)^2 - 4T_1^2]^{\frac{1}{2}} = 2[(h^2 - b^2) - 2b^2 i\delta]^{\frac{1}{2}} \tag{17}$$

We may express the result of taking the square root in (17) in two ways

$$\text{Case I} \quad h > b \quad 2((h^2 - b^2)^{\frac{1}{2}} - b^2 i\delta(h^2 - b^2)^{-\frac{1}{2}}) \tag{18}$$

$$\text{Case II} \quad h < b \quad 2(-b^2\delta(b^2 - h^2)^{-\frac{1}{2}} + i(b^2 - h^2)^{\frac{1}{2}}) \tag{19}$$

In obtaining these expressions expansion by the binomial theorem was used, neglecting higher order terms.

If we treat first Case I, and insert (18) as the value of the radical in (3), we obtain, setting $k^2=1-2h$

$$R=(1/2b)\{2h+b^2-2(h^2-b^2)^{\frac{1}{2}}+2b^2\delta^2(h^2-b^2)^{-\frac{1}{2}}$$
$$-i\delta(2h-b^2-2(h^2-b^2)^{\frac{1}{2}}-2b^2(h^2-b^2)^{-\frac{1}{2}}\} \tag{20}$$

Now if δ is small, the real part of R will be much greater than the imaginary part, and we obtain

$$I=(1/b^2)(h-(h^2-b^2)^{\frac{1}{2}})^2=(h/b-[(h^2/b^2)-1]^{\frac{1}{2}})^2 \tag{21}$$

In Case II, we obtain for R

$$R=(1/2b)\{2h+b^2+2b^2\delta(b^2-h^2)^{-\frac{1}{2}}-2\delta(b^2-h^2)^{\frac{1}{2}}$$
$$-i(2h\delta-b^2\delta+2b^2\delta^2(b^2-h^2)^{\frac{1}{2}}+2(b^2-h^2)^{\frac{1}{2}}\} \tag{22}$$

Neglecting higher order terms, this gives

$$R=(1/2b)(2h-2i(b^2-h^2)^{\frac{1}{2}}) \text{ and } I=1 \tag{23}$$

Thus in Case II the intensity of the reflected beam will differ from that of the incident only by very small quantities. This means practically 100% reflection under the ideal conditions postulated.

Neither of the results (22) or (23) are valid if h and b are so nearly equal that terms in their cubes and higher powers are not negligible in comparison with $\pm(h^2-b^2)$. Nevertheless it is possible to evaluate I if $h=b$, thus obtaining a point in this region. It is easily shown that here the intensity of reflection, as in Case II, will differ from unity only by very small quantities.

Case II, $b>h$, is the most important, as at the wave-lengths ordinarily used, the crystals widely used in x-ray spectroscopy have $b>h$. The result of perfect reflection from a perfect crystal at the maximum of the "rocking curve" for this case has previously been obtained by Darwin and Ewald. The result of Case I, $b<h$, might possibly be of interest in the reflection of very soft x-rays from crystals containing heavy atoms.

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