

## THEORY OF THE DOUBLE X-RAY SPECTROMETER

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## ABSTRACT

The geometric factors in the construction and use of the double x-ray spectrometer are examined in detail. It is found that the resolution of the instrument is not affected by the width of the slits but that, on the other hand, the height of the slits must be limited to preserve resolution. A formula is given for the limiting value of the ratio—average height of effective slits: distance between effective slits—for any particular width of observed line, in order that the width observed be the result principally of the physical factors. The physical factors, namely, crystal imperfection, line width, diffuseness of absorption limits, are also discussed and formulas are derived by means of which the experimental curves found with the instrument may be interpreted physically.

IN RECENT work of Bergen Davis, Slack and Purks on various problems involving a high resolution in the x-ray region they have made use of the double x-ray spectrometer. The instrument is essentially an ordinary spectrometer with the addition of a second crystal which may be turned through accurately measured small angular intervals. It is described in sufficient detail in the papers of Davis and Slack<sup>1</sup> and Davis and Purks.<sup>2,3</sup> The arrangement had been used by Davis and Stempel<sup>4</sup> in their classic measurement of the efficiency of reflection of crystals. Ehrenberg and Mark<sup>5</sup> have also used this arrangement for work similar to that of Davis and Purks.

The present paper is the result of an attempt to determine theoretically the various factors which should be taken into account in the use of the instrument, and to deduce the relations which exist between the characteristics of the radiation entering the instrument, the perfection of the crystals, and the curves found experimentally by means of the instrument. It may be considered as an extension of the work of Richtmyer,<sup>6</sup> since it attempts to develop for the double spectrometer relations similar to those he developed (graphically) for the single crystal instrument.

This discussion is divided into three parts. Part I deals with the effect of poor adjustment of the crystals as to verticality and with the effect of finite slit dimensions. The argument in this part is based upon the assumption of geometrically ideal Bragg reflectors. The results of Part I are therefore not directly applicable to the real situation. Part II is a discussion of the effects of real crystals and real radiation. Relations are found for various types of entering radiation connecting the form of the observed curves with the actual wave-length distribution. In Part III the condition which the slit heights must fulfill in order that the results of Part II may be applied is given. The application of those results to the work of Davis and Purks is then discussed.

## I. GEOMETRICAL

We set ourselves the problem of finding the relations which must be satisfied by the directional coordinates of an incoming ray of wave-

length  $\lambda$  in order that it may be reflected from both crystals. The geometric situation is rather complicated and it seems simpler to derive a vector equation first, and then to translate it into angular notation.

In Fig. 1  $AB$  and  $CD$  are the traces on the  $xy$  or horizontal plane of two idealized Bragg reflectors mounted so that by rotating the supports of either or both, the angle  $\beta$  between these traces may be varied. The vector  $\mathbf{r}$  is a unit vector in the direction of the incoming ray, the vector  $\mathbf{R}$  is a unit vector in the direction of this ray after the first reflection. The vectors  $\mathbf{n}_1$  and  $\mathbf{n}_2$  are the unit normals drawn out from the two reflecting surfaces. In the figure only the projections of these vectors on the  $xy$  plane are shown. The angles indicated in the figure are angles between horizontal traces and projections only. The  $x$  axis makes the angle  $\theta_1$  with  $AB$  and the line  $EF$  makes the angle  $\theta_2$  with  $CD$ . These angles are the Bragg angles for the reflection under consideration. The angle  $\omega$  is the angle between the horizontal projection of  $\mathbf{r}$  and the  $x$  axis. The angle  $\epsilon$  is the angle between the horizontal projection of  $\mathbf{R}$  and  $EF$ . Angles not shown in the figure but readily visualized are: the angle  $\psi$  between  $\mathbf{r}$  and its horizontal projection, the angle  $\delta_1$  between  $\mathbf{n}_1$  and its horizontal projection, and the angle  $\delta_2$  between  $\mathbf{n}_2$  and its horizontal projection. The  $z$  axis is to be considered as coming out of the plane of the figure.

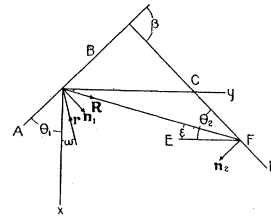


Fig. 1.

The conditions for reflection of the incoming ray from the first crystal may be written

$$\mathbf{r} \cdot \mathbf{n}_1 = -\sin \theta_1 = -p_1 \lambda / 2d ; \mathbf{r} \cdot \mathbf{n}_1 = -\mathbf{R} \cdot \mathbf{n}_1 ; \mathbf{r} \times \mathbf{n}_1 = \mathbf{R} \times \mathbf{n}_1. \quad (1)(2)(3)$$

where  $p_1$  is the order of the first reflection and  $d$  the crystal lattice constant. In order that the ray reflected from the first crystal be again reflected from the second, at order  $p_2$ , we must have

$$\mathbf{R} \cdot \mathbf{n}_2 = -\sin \theta_2 = -p_2 \lambda / 2d = p_2 \mathbf{r} \cdot \mathbf{n}_1 / p_1 \quad (4)$$

By operating upon both members of Eq. (3) with  $\mathbf{n}_1 \times$ , expanding the triple product and substituting from Eq. (2), we obtain

$$\mathbf{R} = \mathbf{r} - 2\mathbf{r} \cdot \mathbf{n}_1 \mathbf{n}_1 \quad (5)$$

By operating upon both members of Eq. (5) with  $\mathbf{n}_2 \cdot$ , and using Eq. (4) we derive

$$p_1 \mathbf{r} \cdot \mathbf{n}_2 - 2p_1 \mathbf{r} \cdot \mathbf{n}_1 \mathbf{n}_1 \cdot \mathbf{n}_2 = p_2 \mathbf{r} \cdot \mathbf{n}_1 \quad (6)$$

an equation which with Eq. (1) expresses the condition for the double reflection of the incoming ray.

In order that these equations may be of further use it is necessary that they be rewritten in terms of the direction coordinates of the vectors involved. The following equations are easily seen to be a consequence of our definitions of the angles involved, with the added consideration that all powers of  $\delta_1$  and  $\delta_2$  above the first are neglected.

$$\begin{aligned}
r_x &= -\cos \psi \cos \omega & n_{1x} &= \sin \theta_1 & n_{2x} &= \sin (\theta_1 + \beta) \\
r_y &= -\cos \psi \sin \omega & n_{1y} &= \cos \theta_1 & n_{2y} &= \cos (\theta_1 + \beta) \\
r_z &= -\sin \psi & n_{1z} &= \delta_1 & n_{2z} &= \delta_2
\end{aligned} \tag{7}$$

With the help of Eqs. (7), we may write Eq. (6) in trigonometric form. Noting Eq. (1) we get

$$p_1 \cos \psi \sin (\omega + \theta_1 + \beta) + p_1 \delta_2 \sin \psi - 2p_1 \sin \theta_1 \cos \beta = p_2 \sin \theta_1 \tag{8}$$

Eq. (1) may be written in angular notation as

$$\cos \psi \sin (\omega + \theta_1) = \sin \theta_1 - \delta_1 \sin \psi \tag{9}$$

or

$$\cos \psi \cos (\omega + \theta_1) = (\cos^2 \psi + 2\delta_1 \sin \theta_1 \sin \psi - \sin^2 \theta_1)^{1/2} \tag{10}$$

Noting the identity

$$\sin (\omega + \theta_1 + \beta) = \sin \beta \cos (\omega + \theta_1) + \cos \beta \sin (\omega + \theta_1)$$

we may substitute from Eqs. (9) and (10) in Eq. (8) and get

$$\sin \beta (\cos^2 \psi + 2\delta_1 \sin \theta_1 \sin \psi - \sin^2 \theta_1)^{1/2} - \cos \beta (\sin \theta_1 + \delta_1 \sin \psi) = \sin \theta_2 - \delta_2 \sin \psi \tag{11}$$

Introduce the angles  $\gamma$  and  $\eta$  such that

$$\sin \beta \cos \gamma - \cos \beta \sin \gamma = \sin \eta \tag{12}$$

Comparing Eqs. (11) and (12) and neglecting terms in  $\psi$  of degree above the second, as well as those in  $\delta$  higher than the first, we have

$$\gamma = \sin^{-1} (\sin \theta_1 + \delta_1 \psi - 2 \sin^2 \theta_1 \delta_1 \psi + \frac{1}{2} \sin \theta_1 \psi^2) \tag{13}$$

$$\eta = \sin^{-1} (\sin \theta_2 - \delta_2 \psi - 2 \sin \theta_1 \sin \theta_2 \delta_1 \psi + \frac{1}{2} \sin \theta_2 \psi^2) \tag{14}$$

Expanding arcsin by Taylor's theorem about  $\sin \theta_1$  and  $\sin \theta_2$  respectively, we obtain

$$\gamma = \theta_1 + \delta_1 \psi / \cos \theta_1 - 2 \sin \theta_1 \tan \theta_1 \delta_1 \psi + \frac{1}{2} \tan \theta_1 \psi^2 \tag{15}$$

$$\eta = \theta_2 - \delta_2 \psi / \cos \theta_2 - 2 \sin \theta_1 \tan \theta_2 \delta_1 \psi + \frac{1}{2} \tan \theta_2 \psi^2 \tag{16}$$

Evidently, from Eq. (12)  $\sin(\beta - \gamma) = \sin \eta$ , which yields the two solutions

$$\beta - \eta - \gamma = 0 : \quad \beta - \pi + \eta - \gamma = 0 \tag{17}(18)$$

These solutions may be written, using Eqs. (15) and (16),

$$M\psi^2 + R\psi = \Delta \tag{19}$$

where  $\Delta = \beta - [\theta_1 + \pi/2 \pm (\theta_2 - \pi/2)]$  representing the angular deviation of the position of the second crystal from the position for reflection of a horizontal ray of wave-length  $\lambda$  entering along the  $x$  axis,  $R = \delta_1 / \cos \theta_1 + \delta_2 / \cos \theta_2 -$

<sup>1</sup> These series will not be convergent even for small values of  $\psi$  if the orders of reflection are so great that the functions of the  $\theta$ 's entering in the  $\psi$  and  $\delta$  terms are very large. For orders used in practice this restriction is unimportant.

$2 \sin \theta_1(\tan \theta_1 \pm \tan \theta_2)\delta_1$  or, by an obvious approximation  $R = \delta_1 + \delta_2^2$  representing the sum or difference of the angles of inclination of the crystals to the vertical, and  $M = \frac{1}{2}(\tan \theta_1 \pm \tan \theta_2)$ , the upper signs being taken when the crystals are in the position of Case I, Fig. 2, in which the ray incident on the first crystal and the ray reflected from the second crystal lie on the same side of the ray reflected from the first crystal; the lower signs being taken when the crystals are in the position of Case II, Fig. 2, in which the first incident and the last reflected rays are on opposite sides of the first reflected ray.

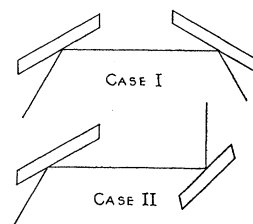


Fig. 2.

The angle  $\Delta$  which determines the position of the second crystal is thus seen to be independent of  $\omega$ ,<sup>3</sup> the angle whose limits are fixed by the horizontal width of the slits, but does depend upon  $\psi$ , the angle whose limits are fixed by  $s$ , the average vertical height of the effective slits and  $L$ , the distance between the effective slits. Evidently

$$-s/L < \psi < s/L \tag{20}$$

We now proceed to find the relation between the angle  $\Delta$  and the energy reflected by the second crystal. We may suppose that the energy coming through the slits at the angle  $\psi$  is a function of that angle. If we denote by  $I(\psi)$  a quantity proportional to the energy of the beam making the angle  $\psi$  with the horizontal plane, then, whatever the form of this function,

$$I(\psi) = 0 \text{ for } |\psi| \geq s/L. \tag{21}$$

Eq. (19) has two solutions for every value of  $\Delta$ . We denote these values of  $\psi$  by  $\psi_1$  and  $\psi_2$ . If  $I_\Delta$  is proportional to the energy coming through after the second reflection, we may write

$$I_\Delta = I(\psi_1) + I(\psi_2), \tag{22}$$

In Fig. 3a the parabolas are the graphs of Eq. (19) for various values of  $R$ . Fig. 3b gives the corresponding curves relating  $I_\Delta$  and  $\Delta$  if  $I(\psi) = s/L - |\psi|$  for  $|\psi| < s/L$ , physically realized if the effective slits are equal in height and the source uniform. If the effective slits differ very much in height, then for  $|\psi| < s/L$ ,  $I(\psi) = \text{constant}$ . The relations between  $I_\Delta$  and  $\Delta$  are obvious from Eq. (22). The curves of Fig. 3a are drawn on the assumption that both  $R$  and  $M$  are positive. If  $R$  were negative the effect would be merely to invert the scale of  $\psi$ , i.e., make it positive downward. Since in ordinary cases  $I(\psi)$  depends only on the absolute value of  $\psi$ , the distribution would be unchanged. If  $M$  were negative the effect would be an inversion of the

<sup>2</sup> There is no pretense at accuracy in this equation. It merely serves to give a rough interpretation of  $R$ . For the further argument all we need say is that  $R$  is not a function of  $\psi$  or  $\omega$  and may be made as small as we please by proper choice of  $\delta_1$  and  $\delta_2$ .

<sup>3</sup> Except that  $\omega$  must be so limited that  $\omega + \theta_1 < \pi/2$ . Practically, for orders of reflection used in practice, this condition is automatically fulfilled because of limitation of crystal size. The reason for this condition lies in the selection of signs in Eqs. (9) and (10).

scale of  $\Delta$ , i.e., positive to the left. The distributions would thus simply be reversed in  $\Delta$ .

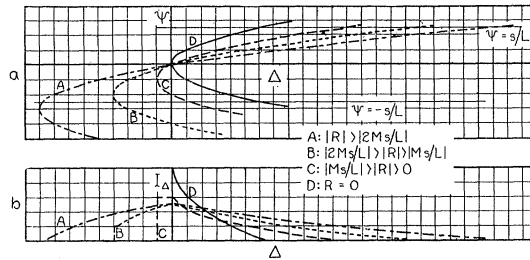


Fig. 3. (a) Graph of Eq. (19) for various values of  $R$ .  $\psi$  is the ordinate,  $\Delta$  the abscissa. (b) Corresponding curves relating  $I_{\Delta}$  and  $\Delta$ .

A consideration of the geometry of the curves of Fig. 3a shows that the maximum width of the curves for  $I_{\Delta}$  may be expressed by the relations

$$W = 2Rs/L \text{ for } R > 2Ms/L \tag{23}$$

and

$$W = Ms^2/L^2 + Rs/L + R^2/4M \text{ for } R < 2Ms/L$$

where  $R$  and  $M$  are always to be taken positively. These equations may be transformed into more practical units. If  $R'$  denotes the value of  $R$  expressed in minutes of arc, and  $W''$  denotes the value of  $W$  expressed in seconds of arc, we have, approximately

$$W'' = 120R's/L \text{ for } R' > 7 \cdot 10^3 Ms/L \tag{24}$$

$$W'' = 2 \cdot 10^5 Ms^2/L^2 + 60R's/L + 4 \cdot 10^3 R'^2/M \text{ for } R' < 7 \cdot 10^3 Ms/L$$

$R'$  and  $M$  again being taken positively.

Fig. 4 shows the graph of  $W''$  and  $R'$  for various values of  $s/L$  and  $M$ . It is obvious from the figure that the most accurate adjustment of  $R'$ , which

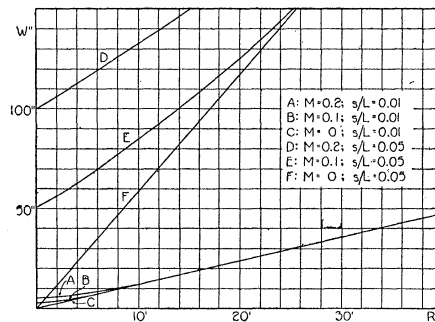


Fig. 4. The geometric width as a function of  $R$ , the deviations from true verticality.

determines the verticality of the crystals, may be made by adjusting  $R'$  for the narrowest curves, when  $s/L$  is large. Furthermore, for  $M \neq 0$ , the value of  $W$  remains greater than zero for all values of  $R$ . The quantity  $W''$  represents only the width due to "geometric" causes. We have assumed that our

crystals are ideal Bragg reflectors and, at least in the non-parallel case, that the radiation is ideally monochromatic. Actually, of course, this is not the case. In fact, the minimum observed widths are all considerably larger than the value of  $W''$  for  $R=0$ , and reasonable values of  $M$  and  $s/L$ . The widths of the observed curves, when adjusted, is therefore principally due to the "physical" causes enumerated above. We may, for this reason, in our discussion of physical causes neglect the geometric width, as soon as  $R'$  and  $s/L$  are properly adjusted. This may be done readily. For a given value of  $M$  it is only necessary to make  $s/L$  large and adjust  $R'$  for minimum width of observed line. The observed width will then be largely "geometrical." If, now,  $s/L$  is decreased so that the value of  $W''$  from Eq. (24) for  $R'=0$  is small compared to the observed width at that setting, our instrument is in such adjustment that the line width observed is principally due to "physical" causes.

It is important to note that, because of the change of sign in the definition of  $R$ , between Case I and Case II, an adjustment for verticality in one case cannot be relied upon for the other, no matter how accurately the crystal mountings are designed.

## II. PHYSICAL

The results of the last section show that the width of the observed lines which may be ascribed to the geometric arrangement of the system may, under reasonable conditions, be made very small. Under the best experimental conditions, however, the actual observed widths are much greater. Their source lies in the fact that we are dealing with real crystals and with radiation of finite wave-length range.

Consider the case in which the rays are ideally monochromatic, but the crystals real. Giving  $\omega$  the same meaning as in Part I, Fig. 1, we may set the energy of the beam after reflection from the first crystal as proportional to  $A_1 e^{-k_1 \omega^2}$ , if  $\theta_1$  of Fig. 1 is the Bragg angle corrected for refraction of the wave-length in question. The justification of this relation rests upon the following:

1. For a perfect crystal the distribution predicted by Ewald and Darwin is shown by the solid line in Fig. 5. The distribution we assume may, by proper choice of  $A$  and  $k$ , be made to fit this reasonably well as shown by the dotted curve in Fig. 5.

2. For an imperfect crystal reflection must be considered as coming from a large number of microcrystals arranged about a mean position. The Gaussian probability function is the most likely distribution.

If  $\theta_2$  is the corrected Bragg angle for the second reflection, and  $\epsilon$  has the meaning for the second reflection which  $\omega$  has for the first, we have, from Eqs. (17) and (18)

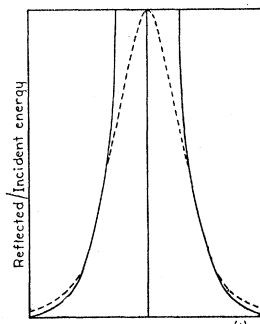


Fig. 5.

$$\text{for Case I ;} \quad \theta_2 - \epsilon = \beta - \theta_1 - \omega \quad (25)$$

$$\text{for Case II :} \quad \theta_2 - \epsilon = \beta - \pi - \theta_1 - \omega \quad (26)$$

$\omega$  and  $\epsilon$  here represent the deviations of the actual reflected ray from the position of the ray reflected by an ideal Bragg reflector.

$A_2 e^{-k_2 \epsilon^2}$  represents a function of  $\epsilon$  proportional to the fraction of the incident energy reflected by the second crystal. The ratio of the total energy getting through both crystals, to that incident on the first will be the product of the corresponding ratios for each crystal, i.e.,

$$F = A_1 A_2 e^{-(k_1 \omega^2 + k_2 \epsilon^2)} \quad (27)$$

If we denote by  $\alpha$  the position of the second crystal as measured from its ideal position, we have

$$\text{for Case I :} \quad \alpha = \beta - \theta_1 - \theta_2 \quad (28)$$

$$\text{for Case II :} \quad \alpha = \beta - \pi - \theta_1 + \theta_2 \quad (29)$$

Combining the last five equations we obtain

$$F = A_1 A_2 e^{-[k_1 \omega^2 + k_2 (\alpha - \omega)^2]} \quad (30)$$

and, since  $\omega$  has a wide range, the total energy coming through at  $\alpha$  will be proportional to

$$J = \int_{-\infty}^{+\infty} F d\omega \quad (31)$$

Integrals of this type may be evaluated as follows:

$$\int_{-\infty}^{+\infty} e^{-[ax^2 + b(y-cx)^2]} dx = [\pi / (bc^2 + a)]^{1/2} e^{-aby^2 / (bc^2 + a)} \quad (32)$$

so that

$$J = A_1 A_2 [\pi / (k_1 + k_2)]^{1/2} e^{-k_1 k_2 \alpha^2 / (k_1 + k_2)} \quad (33)$$

For parallel crystals  $\theta_1 = \theta_2$  and hence by Eq. (29)  $\alpha$  is independent of the wave-length. Under any other conditions  $\alpha$  depends on  $\theta_1$  and  $\theta_2$  and hence upon the wave-length. Suppose that the radiation entering the spectrometer be polychromatic, and that the distribution of energy with the wave-length be described by a function  $f(\lambda - \lambda_0)$  where  $\lambda_0$  is a unique wave-length peculiar to the distribution (center of line, absorption edge, etc.). The energy coming through at any position of the second crystal is evidently proportional to

$$A_1 A_2 [\pi / (k_1 + k_2)]^{1/2} \int_{-\infty}^{+\infty} f(\lambda - \lambda_0) e^{-k_1 k_2 \alpha^2 / (k_1 + k_2)} d\lambda \quad (34)$$

By definition, Eqs. (28) and (29),  $\alpha$  is the deviation of the position of the second crystal from the ideal position for the wave-length considered. If  $\alpha_c$  represents the same deviation as measured from the ideal position for  $\lambda_0$

$$\alpha = \alpha_c - (\lambda - \lambda_0) d(\theta_1 \pm \theta) / d\lambda \quad (35)$$

the upper sign being taken for Case I, and the lower for Case II. Denoting  $k_1 k_2 / (k_1 + k_2)$  by  $K_c$  and  $d(\theta_1 + \theta_2) / d\lambda$  by  $r$  the expression (34) becomes

$$A_1 A_2 \pi^{1/2} / r (k_1 + k_2)^{1/2} \int_{-\infty}^{+\infty} f[(\alpha_c - \alpha) / r] e^{-K_c \alpha^2} d\alpha \quad (36)$$

For the case of line radiation we may assume

$$f(\lambda - \lambda_0) = E e^{-K_\lambda (\lambda - \lambda_0)^2} \quad (37)$$

Substituting in Eq. (36) and using Eq. (32), we obtain

$$J_{\alpha_c} = \frac{\pi E A_1 A_2}{[(K_c r^2 + K_\lambda)(k_1 + k_2)]^{1/2}} e^{-K_c K_\lambda \alpha_c^2 / (K_\lambda + K_c r^2)} \quad (38)$$

For the case of continuous radiation we have, for the small ranges under consideration  $f(\lambda - \lambda_0) = C$ . For this case Eq. (36) becomes

$$J_{\alpha_c} = C A_1 A_2 \pi / r [K_c (k_1 + k_2)]^{1/2} \quad (39)$$

For the case of an absorption edge we may set

$$f(\lambda - \lambda_0) = B + (1/h_a) \int_{-\infty}^{\lambda - \lambda_0} (A - B) e^{-\pi x^2 / h_a^2} dx \quad (40)$$

A graph of this equation is shown in Fig. 6. The quantity  $h_a$  has the significance shown in the figure, and may be used as a measure of the diffuseness of the absorption edge. In this case Eq. (36) becomes

$$J_{\alpha_c} = \frac{A_1 A_2 \pi^{1/2}}{r (k_1 + k_2)^{1/2}} \left[ \int_{-\infty}^{+\infty} B e^{-K_c \alpha^2} d\alpha + \frac{1}{h_a} \int_{-\infty}^{+\infty} e^{-K_c \alpha^2} \int_{-\infty}^{(\alpha_c - \alpha) / r} (A - B) e^{-\pi x^2 / r^2 h_a^2} dx d\alpha \right]$$

so that

$$\frac{dJ_{\alpha_c}}{d\alpha_c} = \frac{A_1 A_2 \pi^{1/2} (A - B)}{r^2 h_a (k_1 + k_2)^{1/2}} \int_{-\infty}^{+\infty} e^{-[K_c \alpha^2 + \pi (\alpha - \alpha_c)^2 / r^2 h_a^2]} d\alpha$$

and, by Eq. (32)

$$\frac{dJ_{\alpha_c}}{d\alpha_c} = \frac{A_1 A_2 \pi (A - B)}{r [(\pi + K_c r^2 h_a^2)(k_1 + k_2)]^{1/2}} e^{-\pi K_c \alpha_c^2 / (\pi + K_c r^2 h_a^2)}$$

giving

$$\left( \frac{dJ_{\alpha_c}}{d\alpha_c} \right)_{\alpha_c = \alpha} = \frac{A_1 A_2 \pi (A - B)}{r [(\pi + K_c r^2 h_a^2)(k_1 + k_2)]^{1/2}} \quad (41)$$

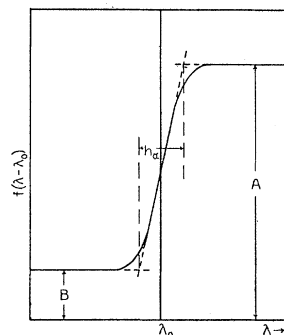


Fig. 6. Graph of Eq. (40).

From Eq. (39) it is evident that the ordinates of the observed curve far on either side of the absorption edge will be  $A A_1 A_2 \pi / r [K_c (k_1 + k_2)]^{1/2}$  and  $B A_1 A_2 \pi / r [K_c (k_1 + k_2)]^{1/2}$ , so that the observed angular width will be



$$h = \frac{(A-B)\pi A_1 A_2}{r [K_c(k_1+k_2)]^{1/2}} \div \left( \frac{dJ_{\alpha_c}}{d\alpha_c} \right)_{\alpha_c=\alpha}$$

Using Eq. (41) this becomes

$$h = (\pi/K_c + r^2 h_a^2)^{1/2}$$

For the probability distributions of Eqs. (30), (33), (37), and (38) we may use as a measure of the width, that at half-maximum energy, which may be expressed as  $2(\log 2)^{1/2}/K^{1/2}$  where  $K$  is the constant of the exponent. If  $H_1$  and  $H_2$  represent these widths for each of the crystals for ideally collimated and monochromatic radiation, we have, using appropriate subscripts, from Eq. (33)

$$H_c = (H_1^2 + H_2^2)^{1/2} \quad (43)$$

or, if the crystals are alike

$$H_c = \sqrt{2} H_1 \quad (44)$$

If the crystals are not parallel the observed angular width  $H_{n,p}$  for a line will be, from Eqs. (37) and (38)

$$H_{n,p} = (H_c^2 + r^2 H_\lambda^2)^{1/2} \quad (45)$$

If the crystals are parallel, the observed angular width  $H_p$  will be

$$H_p = H_c \quad (46)$$

evidently independent of the type of radiation. From Eqs. (42), (43), and (46), the actual width  $h_a$  of an absorption edge, in wave-length units is related to the observed angular width  $h$  and the resultant width for the two crystals at the orders used,  $H_c$ , in the following manner:

$$r^2 h_a^2 = h^2 - \pi H_c^2 / 4 \log 2 = h^2 - 1.13 H_c^2 \quad (47)$$

The quantity  $r$  in the above equations may be expressed as

$$r = d(\theta_1 \pm \theta_2) / d\lambda = p_1 / 2d \cos \theta_1 \pm p_2 / 2d \cos \theta_2 \quad (48)$$

The results expressed by Eqs. (43) to (46) have already been published by Ehrenberg and Mark<sup>5</sup> for the case  $\theta_1 = \theta_2$ . The results here are more general and may be applied even to the case of two crystals of different material.

### III. APPLICATION

The results of Part II may be applied only if the "geometric" width given by Eq. (23) is small compared to the measured widths,  $H_p$ ,  $H_{n,p}$ , or  $h$ . This limitation may be expressed in the following way:

$$\frac{s}{L} \ll \left( \frac{\text{angular width measured}}{\frac{1}{2}(\tan \theta_1 \pm \tan \theta_2)} \right)^{1/2}$$

the upper sign being taken for case I, and the lower for case II. It is, of course, assumed that the adjustment for verticality has been taken care of.

In all the work of Davis and Purks<sup>3</sup> this limitation has been taken into consideration. These authors have recently shown<sup>3</sup> that the natural width of the  $K\alpha$  line of Mo is of the order of 0.1 X-unit. In that work they made use of the equation of Ehrenberg and Mark<sup>5</sup> corresponding to our Eq. (45).

It is of interest to apply Eq. (44) to the data there given. They found with both crystals parallel and reflection at second order  $H_p = 3.75''$ , which gives  $H_1 = 2.65''$ . The corresponding quantity at first order would be twice as great<sup>6</sup> or  $5.4''$  which is to be compared with the value  $5.8''$  given by Compton<sup>7</sup> for a perfect crystal. The result indicates a high order of perfection for the calcite crystals used. If we adopt the value for  $H_1$  at first order as  $5.4''$  we can calculate the breadth of an absorption edge from unpublished data of Davis and Purks. They find for the Mo  $K$  limit  $h = 32'' = 1.6 \times 10^{-4}$  radians at first order on both crystals of calcite, reflecting as in case I. From Eq. (48)  $r = 0.33$  (A-units)<sup>-1</sup>, from Eq. (44)  $H_c = 7.5'' = 3.7 \times 10^{-5}$  radians, and hence, from Eq. (47),  $h_a = 4.65 \times 10^{-4}$  A-units.

This result is to be compared with the upper limit for the width of the Ag  $K$  absorption edge given by Richtmyer<sup>8</sup> as 0.0002 A-units.

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<sup>1</sup> Davis and Slack, Phys. Rev. **27**, 18 (1926).

<sup>2</sup> Davis and Purks, Proc. Nat. Acad. Sci. **13**, 419 (1927).

<sup>3</sup> Davis and Purks, Proc. Nat. Acad. Sci. **14**, 172 (1928).

<sup>4</sup> Davis and Stempel, Phys. Rev. **17**, 608 (1921).

<sup>5</sup> Ehrenberg and Mark, Zeits. f. Physik **42**, (1927).

<sup>6</sup> C. G. Darwin, Phil. Mag. **27**, 675 (1914).

<sup>7</sup> A. H. Compton, X-rays and Electrons, p. 140.

<sup>8</sup> F. K. Richtmyer, Phys. Rev. **26**, 724 (1925).