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## PHYSICAL REVIEW.

# THE GEOMETRY OF IMAGE FORMATION IN X-RAY ANALYSIS.

#### By Horace Scudder Uhler.

*Introduction.*—The theory of diffraction as applied to ordinary surface gratings and to the design of apparatus used in the spectroscopy of radiations having wave-lengths much greater than those of X-rays has been thoroughly worked out, and the most important results obtained are clearly presented in various places, for example, in Kayser's Handbuch der Spectroscopie. The theory of plane space-gratings (rigid crystals) has also been investigated by Laue and Bragg. On the other hand, as far as I have been able to ascertain, from a fairly complete search of the accessible literature of the subject, very little has been published on the general theory upon which the construction of X-ray spectrometers and spectrographs should be based. Accordingly, it may not be superfluous to present the results of my analytical study of some of the questions which arose both during the time when Dr. C. D. Cooksey and I were working on the high frequency spectrum of gallium and later when we were engaged in designing a new X-ray spectrograph for the accurate determination of the wave-lengths of characteristic radiations. Since these wave-lengths are too short to produce diffraction patterns of sensible dimensions, the problems fall within the domain of geometrical optics. As the interference and reflection methods used respectively by Laue and by Bragg lead, of necessity, to the same conclusions, and since the second point of view is the more advantageous for the present purposes, the crystals will be treated as aggregates of reflecting planes throughout the paper. The grating-space of the crystal, the wave-length of the rays, and the order of the spectrum will be considered as constants so that the glancing-angle  $\gamma$  will also be constant, conformably to the well-known relation  $m\lambda = 2d \sin \gamma$ .

General Equations.—Since a material space-lattice consists of a number

#### HORACE SCUDDER UHLER.

of parallel planes of regularly spaced atoms, a first approximation to the case of a real crystal may be made by studying the properties of a single plane of unlimited area which reflects rays of a given wave-length at a constant glancing-angle  $\gamma$ . Accordingly, the first question for consideration will be: To find the general equations of a ray reflected from a perfectly selective mirror when the position and direction of the incident ray are given in terms of certain convenient parameters.

Let the incident ray SI (Fig. 1) be determined by the point  $S(x_1, y_1, z_1)$ 



and the angles  $\alpha$  and  $\beta$ .  $\alpha$  is the angle which the orthogonal projection of the incident ray on the plane XOY makes with the negative direction of the axis  $\overrightarrow{OY}$ .  $\beta$  is the angle which the ray  $\overrightarrow{SI}$  forms with this projection. Hence,  $\alpha$  and  $\beta$  may be looked upon as giving the azimuth and altitude of the incident ray, respectively. The mirror MO may rotate

around  $\overline{OZ}$  as axis.  $\theta$  is the angle made by any normal to the mirror (such as  $\overline{ON}$ ) with the coördinate plane XOZ. I (x', y', z') denotes the point of incidence, and  $\overline{IR}$  indicates the reflected ray. The equation of the reflector is

$$\cos \theta \cdot x + \sin \theta \cdot y = 0. \tag{I}$$

By spherical trigonometry (or otherwise) it is easy to show that the direction cosines of the incident ray are sin  $\alpha \cos \beta$ ,  $-\cos \alpha \cos \beta$ , and sin  $\beta$ . Hence, the equations of this ray are

$$\frac{x-x_1}{\sin \alpha \cos \beta} = -\frac{y-y_1}{\cos \alpha \cos \beta} = \frac{z-z_1}{\sin \beta}.$$
 (2)

From equations (1) and (2) the coördinates of the point of incidence I are found to be

$$x' = \frac{(x_1 \cos \alpha + y_1 \sin \alpha) \sin \theta}{\sin (\theta - \alpha)},$$
  

$$y' = -\frac{(x_1 \cos \alpha + y_1 \sin \alpha) \cos \theta}{\sin (\theta - \alpha)},$$
  

$$z' = z_1 + \frac{(x_1 \cos \theta + y_1 \sin \theta) \tan \beta}{\sin (\theta - \alpha)}$$
(3)

SECOND SERIES.

Let l, m, and n denote the direction cosines of the reflected ray so that the equations of this line may be written

$$\frac{x - x'}{l} = \frac{y - y'}{m} = \frac{z - z'}{n}.$$
 (4)

Since directions alone are now involved, expressions for l, m, and n in terms of  $\alpha$ ,  $\beta$ , and  $\theta$  may be obtained by moving all necessary lines parallel to themselves until they radiate from the center of an auxiliary sphere.

In Fig. 2,  $\overline{OI}$ ,  $\overline{OR}$ , and  $\overline{ON}$  are parallel respectively to the incident



ray, the reflected ray, and the normal to the mirror. The law of reflection requires that  $\angle QOR = \angle POI$  (=  $\beta$ ). Arcs of great circles are drawn through the various points as shown in the diagram.  $\angle Y'OP$ =  $\alpha$ ,  $\angle XON = \theta$ . Let  $\angle QOX \equiv \xi$ .  $\angle IOR = 2\gamma$  = deviation of ray.

In the rt.  $\triangle QNR$ ,

$$\cos\left(\frac{\pi}{2}-\gamma\right)=\cos\beta\cos\left(\theta+\xi\right).$$

In the rt.  $\triangle PNI$ ,

$$\cos\left(\frac{\pi}{2}+\gamma\right) = \cos\beta\cos\left(\theta+\frac{\pi}{2}-\alpha\right)$$

or

 $\sin \gamma = \cos \beta \sin (\theta - \alpha);$ 

hence

$$\xi=\frac{\pi}{2}-(2\theta-\alpha)$$

3

(5)

In the rt.  $\triangle QXR$ ,

 $l = \cos \beta \cos \xi$ 

or

4

$$l = \cos \beta \sin (2\theta - \alpha);$$

In the rt.  $\triangle QYR$ ,

$$m = \cos \beta \cos \left(\frac{\pi}{2} + \xi\right)$$

or

$$m = -\cos\beta\cos\left(2\theta - \alpha\right),\tag{7}$$

$$n = \sin \beta. \tag{8}$$

In general, being given  $\alpha$ ,  $\beta$ , and  $\gamma$  relation (5) furnishes two supplementary values for  $\theta - \alpha$ . Hence the values of  $\theta$  corresponding to the two possible angular positions of the reflecting plane are determined. Having chosen the value of  $\theta$  which is required, or which is compatible with the position of the point S (Fig. 1), l and m are given by formulæ (6) and (7), respectively. Since the coördinates  $x_1$ ,  $y_1$ , and  $z_1$  are also supposed to be known, the values of x', y', and z' may be computed at once from (3). Therefore the six parameters of equations (4) have been theoretically evaluated from the assigned data.

The preceding analysis is pertinent to the theory of the design of X-ray spectrometers in two respects: (a) it facilitates the actual calculation of the position and direction of the reflected ray so that its intersection with a photographic plate, or its path in an ionization chamber, can be predicted from the hypothetical positions of slits, diaphragms, etc.--in particular, spurious images and stray rays can be anticipated and eliminated; and (b) the numbered formulæ may be combined in various ways leading to conditional equations having useful interpretations. It may also be remarked that, as far as my information goes, all the papers which relate to the geometry of "image" formation with plane crystals restrict the problem to two dimensions, or more precisely, to pencils of rays lying in one plane perpendicular to the axis of rotation of the crystal ( $\beta = 0$ ). Although these uniplanar problems are undoubtedly the simplest and most important, nevertheless they afford no information as to what happens when the angular altitude of the rays is not equal to zero. As will appear later, images may be widened unsymmetrically and appreciably, under special circumstances, due to the fact that  $\beta$  is not sufficiently small.

Complete Ray Determined by Two Points.—A solution of the following problem will now be outlined: To find a formula for  $\theta$  being given the value of the glancing-angle  $\gamma$  and the two independent conditions that

SECOND

(6)

the incident and reflected rays shall pass through the fixed points  $(x_1, y_1, z_1)$  and  $(x_2, y_2, z_2)$ , respectively. Equations (4) already satisfy the first condition hence they will involve both conditions when written as

$$m(x_2 - x') = l(y_2 - y'),$$
  

$$n(x_2 - x') = l(z_2 - z').$$

Substitution, in the first equation, of the expressions for x', y', l, and m given by (3), (6), and (7) leads to

$$(x_1 \sin 2\theta - y_1 \cos 2\theta + y_2) \sin (2\theta - \alpha) + (x_1 \cos 2\theta + y_1 \sin 2\theta + x_2) \cos (2\theta - \alpha) = 0.$$
(9)

Similarly, the second equation when combined with (3), (6), and (8) reduces to

$$x_1 \tan \beta \cos 2\theta + y_1 \tan \beta \sin 2\theta + x_2 \tan \beta + (z_1 - z_2) \sin (2\theta - \alpha) = 0.$$
 (10)

Assuming, for the time being, that the trinomial coefficients in (9) do not vanish simultaneously and that (10) is not satisfied by having  $\beta = 0$  and  $z_1 - z_2 = 0$ , the elimination of  $\alpha$  and  $\beta$  from formulæ (5), (9), and (10) may be effected by the following operations. The square of (5) may be transformed into

$$\tan^2\beta = [\sin^2(\theta - \alpha) - \sin^2\gamma] \csc^2\gamma,$$

which is then equated to the expression for  $\tan^2 \beta$  obtained directly from (10). Since  $\theta - \alpha$  is identically the same as  $(2\theta - \alpha) - \theta$  it follows that

$$\sin^2\left(\theta - \alpha\right) = \frac{1}{2}(\tau^2 + \tau^2\cos 2\theta - 2\tau\sin 2\theta + \mathbf{I} - \cos 2\theta)(\mathbf{I} + \tau^2)^{-1},$$

where  $\tau \equiv \tan (2\theta - \alpha)$ . Consequently the equation resulting from the elimination of  $\tan^2 \beta$  may be written as a rational function of  $\tau$ , sin  $2\theta$ , and  $\cos 2\theta$ . Elimination of  $\tau$  is accomplished at once by substitution of  $\tau$  from (9). The equation finally obtained is of the form

$$2A \sin 2\theta + B \cos 2\theta + C = 0,$$

where

$$A \equiv x_1y_1 + x_2y_2 + (x_1y_2 + x_2y_1)\cos 2\gamma,$$
  

$$B \equiv x_1^2 + x_2^2 - y_1^2 - y_2^2 + 2(x_1x_2 - y_1y_2)\cos 2\gamma,$$
  

$$C \equiv 2x_1x_2 + 2y_1y_2 - (z_1 - z_2)^2 + [x_1^2 + x_2^2 + y_1^2 + y_2^2 + (z_1 - z_2)^2]\cos 2\gamma.$$

Since  $\sin 2\theta = 2t(\mathbf{I} + t^2)^{-1}$  and  $\cos 2\theta = (\mathbf{I} - t^2)(\mathbf{I} + t^2)^{-1}$ , where  $\equiv \tan \theta$ , the last equation may be transformed into the following quadratic in the single unknown quantity t

$$at^{2} + 2bt + c = 0,$$

$$a \equiv (y_{1} + y_{2})^{2} \cos^{2} \gamma - [(x_{1} - x_{2})^{2} + (z_{1} - z_{2})^{2}] \sin^{2} \gamma,$$

$$b \equiv (x_{1} + x_{2})(y_{1} + y_{2}) - 2(x_{1}y_{2} + x_{2}y_{1}) \sin^{2} \gamma,$$

$$c \equiv (x_{1} + x_{2})^{2} \cos^{2} \gamma - [(y_{1} - y_{2})^{2} + (z_{1} - z_{2})^{2}] \sin^{2} \gamma.$$
(11)

It should be remarked, in passing, that formula (II) may also be derived by making use of the fact that the reflected ray (extended backward) must pass through the virtual image of the point  $(x_1, y_1, z_1)$ . As formula (II) is of the second degree, the conclusion may be drawn that, in general, not more than two rays can be constructed when one point on the incident segment, one on the reflected segment, and the glancing-angle are given. In applying the quadratic to numerical data it sometimes happens that one of the roots corresponds to a position of the mirror for which the points  $(x_1, y_1, z_1)$  and  $(x_2, y_2, z_2)$  are on opposite sides of the reflecting plane, thus causing one of the points to play the rôle of a virtual image. By equation (I), a necessary and sufficient condition for the points to lie on the same side of the plane is that  $x_1 + ty_1$  and  $x_2 + ty_2$  shall have like signs.

In the special case where both of the given points lie in a plane perpendicular to the axis of rotation  $(z_1 = z_2)$ , the roots of (11) may be reduced to the following rational form

$$t = \mp \frac{(x_1 + x_2) \cos \gamma \mp (y_1 - y_2) \sin \gamma}{(x_1 - x_2) \sin \gamma \pm (y_1 + y_2) \cos \gamma},$$
 (11')

in which the upper signs, or the lower ones, must be taken together.<sup>1</sup>

Point Source and Negligible Penetration.—The special case of rays lying in a plane perpendicular to the axis of rotation of the mirror will next be considered. This condition is represented by  $\beta = 0$  and  $z_1 - z_2$ = 0, hence formula (10) is satisfied irrespective of the (finite) values of  $x_1, x_2, y_1, \alpha$ , and  $\theta$ . The admissible solutions of (5) are now  $\theta_1 = \alpha + \gamma$ and  $\theta_2 = \pi - (\gamma - \alpha)$ . Equation (9) reduces to  $(x \mp y_1 \sin 2\gamma) \cos (2\gamma \pm \alpha) \pm (y + y_1 \cos 2\gamma) \sin (2\gamma \pm \alpha) = 0$ , (12) in which the subscripts 2 have been suppressed.  $x_1$  has been put equal

in which the subscripts 2 have been suppressed,  $x_1$  has been put equal to zero for sake of simplicity, and the upper and lower signs correspond respectively to  $\theta_1$  and  $\theta_2$ . As may be seen at a glance, the lines represented by the upper and lower equations of (12) always pass respectively

<sup>&</sup>lt;sup>1</sup> The order of the signs corresponds to  $t = (-b \pm \sqrt{b^2 - ac})/a$ .

#### GEOMETRY OF IMAGE FORMATION.

through the points  $(\pm y_1 \sin 2\gamma, -y_1 \cos 2\gamma)$  independently of  $\alpha$ . Therefore, all rays lying in a plane perpendicular to the axis of rotation of a plane selective mirror—the axis coinciding with the mirror (pure rotation) and radiating from a single point will, after reflection, pass through two focal points each of which is at the same distance from the axis as the radiant point, the angles of deviation of the axial or principal rays of the pencils being numerically equal to twice the constant glancing-angle. This fundamental theorem is not new, since demonstrations involving only elementary, non-analytic geometry have been given by Bragg, E. Wagner, and others. Nevertheless I have not seen a published proof which involves a concise, formal statement of the special conditions under which the theorem is valid. The limitations may have been fully appreciated, but they seem to have been tacitly assumed.

By taking the sum of the squares of the corresponding members of the equations

 $-x_2 = x_1 \cos 2\theta + y_1 \sin 2\theta,$  $-y_2 = x_1 \sin 2\theta - y_1 \cos 2\theta,$ 

it will be found immediately that

$$x_2^2 + y_2^2 = x_1^2 + y_1^2.$$

Therefore as  $\gamma$  varies, the image point  $(x_2, y_2)$  describes the circumference of the focal circle having the radius  $\sqrt{x_1^2 + y_1^2}$ .

Point Source and Appreciable Penetration.—The qualifying remark, between the dashes in the last italicized sentence, will now receive attention. The pertinence of the question depends on the fact that, in general, X-rays penetrate to a finite depth into the diffracting crystal, so that rigorously not more than one plane of atoms can contain the axis of rotation. If this plane is the mean effective one then the parallel active planes must be situated on both sides of the axis and at different distances from the same. The problem is, accordingly: To investigate the properties of rays lying in a plane perpendicular to the axis of rotation when this axis is parallel to the reflecting surface, but does not coincide with the surface.

In Fig. 3, S(a, o) is the radiant point. The axis of rotation and the plane of the mirror are both perpendicular to the plane XOY, and they intersect it in the point O and the line  $\overline{MN}$ , respectively. Let p symbolize the length of the normal  $\overline{OF'}$  dropped from O on  $\overline{MN}$ , and let this perpendicular make an angle  $\alpha'$  with the direction  $\overline{OX}$ . The equation of the mirror is

 $\cos \alpha' \cdot x + \sin \alpha' \cdot y - p = 0.$ 

SECOND SERIES

The equation of the line joining S to its virtual image S' is

 $y = (x - a) \tan a'$ 

hence, the coördinates of the foot of the perpendicular F dropped from S on  $\overline{MN}$  are





$$x' = p \cos \alpha' + a \sin^2 \alpha',$$
  

$$y' = (p - a \cos \alpha') \sin \alpha'.$$

Since  $\overline{S'F} = \overline{FS}$  the coördinates of S' are found to be

$$x'' = 2p \cos \alpha' - a \cos 2\alpha',$$
  
$$y'' = 2(p - a \cos \alpha') \sin \alpha'.$$

The angle which the reflected ray makes with  $\overline{OX}$  equals  $(\pi/2) + \alpha' - \gamma$ . Therefore the equation of the reflected ray  $\overline{IR}$  is

 $\cos (\alpha' - \gamma) \cdot x + \sin (\alpha' - \gamma) \cdot y + a \cos (\alpha' + \gamma) - 2p \cos \gamma = 0.$  (13) Differentiation of equation (13) with respect to  $\alpha'$  gives

$$\sin (\alpha' - \gamma) \cdot x - \cos (\alpha' - \gamma) \cdot y + a \sin (\alpha' + \gamma) = 0.$$
 (14)

The envelope of the reflected ray is found at once by eliminating  $\alpha'$  from the last two equations. (13) and (14) may be written as

$$A \sin \alpha' + B \cos \alpha' = C$$

and

$$B\sin\alpha' - A\cos\alpha' = 0$$

where

$$A \equiv \sin \gamma \cdot x + \cos \gamma \cdot y - a \sin \gamma,$$
  
$$B \equiv \cos \gamma \cdot x - \sin \gamma \cdot y + a \cos \gamma$$

GEOMETRY OF IMAGE FORMATION.

and

Vol. XI. No. 1.

$$C \equiv 2p \cos \gamma.$$

On squaring and adding the abbreviated equations, it is found that

$$A^{2} + B^{2} = C^{2}$$
$$(x + a\cos 2\gamma)^{2} + (y - a\sin 2\gamma)^{2} = (2p\cos \gamma)^{2}.$$
 (15)

or

Accordingly, the complete envelope is the circumference of a circle having  
the radius 
$$2p \cos \gamma$$
 and its center at the point O'  $(-a \cos 2\gamma, a \sin 2\gamma)$ ,  
which is identical in position with the focal point corresponding to  
 $p = 0$ . Formula (15) suffers no modification when the source S and the  
axis of rotation are on the same side of the mirror, that is, when the axis  
is in front of the reflecting plane instead of behind it.

The general nature and rational form of the preceding equations, together with the unlimited area of the reflecting surface, enable the analytical conditions to be fulfilled by points situated on reversed prolongations of the lines. Such points are formally correct but they do not correspond to the actual paths of the X-rays. As some portions of the envelope may also fail to satisfy the practical requirements of the problem, and since the radius of the circle is not negligible for penetrating radiations, it becomes necessary to examine in detail the properties of this locus.

The coördinates of the point of contact R of the reflected ray with the circle are easily derived from (13) and (15). They are

$$x_{c} = -a \cos 2\gamma + 2p \cos \gamma \cos (\alpha' - \gamma)$$
  

$$y_{c} = a \sin 2\gamma + 2p \cos \gamma \sin (\alpha' - \gamma)$$
(16)

Let  $\phi$  denote the angle made by the radius to the point of contact O'R with the direction  $\overline{OX}$ . Then

$$\tan \phi = \frac{y_c - a \sin 2\gamma}{x_c + a \cos 2\gamma};$$

hence, by (16),  $\tan \phi = \tan (\alpha' - \gamma)$ ; therefore

$$\phi = \alpha' - \gamma.$$

This simple relation is very helpful in following the motion of the point R when that of the point F' is known.

Now let another reflecting plane M'N', which is parallel to MN and at the same numerical distance p from O, be taken into consideration. Assuming  $\gamma$  to have the same value for the plane M'N' as for MN, the coördinates of the point of contact R' may be found either by changing  $\alpha'$  to  $\pi + \alpha'$  or p to -p in formulæ (16). Consequently

$$\frac{1}{2}(x_c + x_c') = -a \cos 2\gamma, \frac{1}{2}(y_c + y_c') = a \sin 2\gamma,$$

and these are the coördinates of the center O' of the envelope. In other words, under the specified conditions, the points of contact are situated at the extremities of the same diameter. It is easy to show that the points S, I, and I' are collinear, so that both reflected rays arise from one incident ray.

A fair approximation to the circumstances pertaining to a real crystal may be made by imagining the space between MN and M'N' to be filled with pairs of symmetrically situated reflecting planes for which pvaries continuously (grating-spaces are of the order  $3 \times 10^{-8}$  cm.) from zero to a maximum value. To each pair of planes will correspond a little circular envelope, so that the entire area enclosed by the largest circumference will be crossed by the X-rays. It is therefore evident that, when the medial effective reflecting plane of the crystal coincides with the axis of rotation, the image of a *point source* will not be displaced laterally with respect to the ideal image O', which corresponds to negligible penetration. On the other hand, if the average reflecting plane is sufficiently eccentric, the image may be displaced enough to influence very accurate experimental work. Obviously, this displacement may be on either side of the axial ray  $\overline{OO'}$ .

Attention should also be called to the radius of the envelope  $2p \cos \gamma$ . As the X-rays become harder (shorter wave-length), not only does the maximum value of p become greater but the glancing-angle  $\gamma$  decreases, thus causing  $\cos \gamma$  to increase. Hence, the radius is increased by both of its variable factors. Theoretically, therefore, this is unfortunate since the images become broader as the experimental difficulties inherent in the usual methods of determining glancing-angles increase.

The preceding analysis and deductions are subject to such qualifications as may arise from the finite width of the crystal face, the distance of the source S from O, etc. For example, by combining the equation of the mirror with formula (13), the coördinates of the point of incidence I are found to be

$$x_i = [p \sin (\alpha' + \gamma) - a \sin \alpha' \cos (\alpha' + \gamma)] \csc \gamma,$$
  

$$y_i = (a \cos \alpha' - p) \csc \gamma \cos (\alpha' + \gamma).$$

The point F' being  $(p \cos \alpha', p \sin \alpha')$ , the distance from F' to I is given

10

by

 $\delta = [p \cos \gamma - a \cos (\alpha' + \gamma)] \csc \gamma. \tag{17}$ 

Evidently the rotation of the crystal must not cause this quantity to vary over a greater range than the width of the face of the crystal.

Broadening of Image by Oblique Rays.—As the effect of the altitude angle  $\beta$  can be illustrated in a very large number of ways it becomes necessary to choose some specific case when quantitative data are desired. Accordingly, the following special problem has been selected for the reasons that it is relatively simple, and that it conforms closely to the experimental conditions which obtain when the ionization method is used, or when the photographic plate is placed normal to the axis of the beam of X-rays.

In Fig. 4, the line  $\overline{ST}$ , parallel to  $\overline{OZ}$ , may be looked upon as a slit of negligible width. Let the point S be (0,  $y_1$ , -h). P indicates any

point on the focal circle (assuming no penetration and no eccentricity) having the radius  $\overline{OT} = y_1$ . By hypothesis, the reflected ray  $\overline{IR}$  is required to pass through  $P(x_2, y_2, 0)$ . In general, as the angle  $\beta$  varies, the point P will move around the circumference of the focal circle, and the arc passed over will correspond to the width of the image which would be recorded on a photographic film



wrapped in the form of a circular cylinder, having  $\overline{OZ}$  for axis and  $y_1$  as radius. Before proceeding to numerical quantities, two simple algebraic relations must be derived.

Since  $x_1 = z_2 = 0$  and  $z_1 = -h$ , formula (10) reduces to

 $x_2 = h \cot \beta \sin (2\theta - \alpha) - y_1 \sin 2\theta$ 

which, when substituted in equation (9), leads to

$$y_2 = y_1 \cos 2\theta - h \cot \beta \cos (2\theta - \alpha).$$

Substitution of these expressions in the equation of the focal circle

$$x_2^2 + y_2^2 = y_1^2$$

gives

$$h = 2y_1 \cos \alpha \tan \beta. \tag{18}$$

II

In order to compare different positions of the point P, as this intersection moves along the circular arc, it is necessary to find a connection between the angle  $Y'OP(\eta)$  and known quantities. Replacing  $h \cot \beta$ by its equal  $2y_1 \cos \alpha$  in the preceding simplified formulæ for  $x_2$  and  $y_2$ , and noting that  $2\theta = (2\theta - \alpha) + \alpha$ , it will be found that

$$x_2 = y_1 \sin 2(\theta - \alpha),$$
  
-  $y_2 = y_1 \cos 2(\theta - \alpha).$ 

But

$$\tan \eta = \frac{x_2}{-y_2}$$

 $\eta = 2(\theta - \alpha).$ 

hence

Therefore, under the given conditions, 
$$\eta$$
 is equal to the deviation of the orthogonal projection on the plane XOY of the ray SIR. (See  $\angle POO$ , Fig. 2).

Finally, by formula (5),

$$\sin \frac{1}{2}\eta = \frac{\sin \gamma}{\cos \beta} \tag{19}^1$$

This equation shows that  $\eta$  has a minimum value when  $\beta = 0$ , hence, for slits of zero width, settings should be made on the *inferior edge* of a photographic image in order to obtain the correct value of the glancing-angle ( $\eta_0 = 2\gamma$ ,  $\beta = 0$ ).

The data for  $\eta_0$ , and h, in Table I., were calculated from the arbitrary values of  $\beta_0$  given in the first column,  $\alpha$  being assigned the value zero throughout. In all cases  $\gamma = 15^{\circ}$  and  $\dot{y}_1 = 10$  cm.

| β₀.    | 70-        | h (mm.) . |  |  |
|--------|------------|-----------|--|--|
| 0° 0′  | 30° 0′ 0″  | 0         |  |  |
| 0° 30′ | 30° 0′ 4″  | 1.745     |  |  |
| 1° 0′  | 30° 0′ 17″ | 3.491     |  |  |
| 1° 30′ | 30° 0′ 38″ | 5.237     |  |  |
| 2° 0′  | 30° 1′ 7″  | 6.984     |  |  |
| 2° 30′ | 30° 1′ 45″ | 8.732     |  |  |
| 3° 0'  | 30° 2′ 32″ | 10.482    |  |  |

TABLE I.

<sup>1</sup> It is interesting to note that this equation is identical in form and meaning with the relation  $\sin \frac{1}{2}D = \sin \frac{1}{2}E \cos \eta_1$  which occurs in the theory of oblique *refraction* through prisms. Therefore, it is an expression of the single fact common to the laws of reflection and single refraction, which is, that the angles of incidence and reflection or refraction lie in the same plane containing the normal. See, H. S. Uhler, On the Deviation Produced by Prisms, Amer. Jour. Science, Vol. 35, p. 389 (1913).

The second column shows quantitatively how the point P (Fig. 4) moves along the circumference as  $\beta_0$  receives equal increments,  $\alpha$  remaining unchanged. The second differences for  $\eta_0$  are practically constant. The third column<sup>1</sup> indicates the point on the slit through which the ray must pass in order to give the corresponding value of  $\eta_0$ .

If the image on a photographic film were of uniform density from one edge to the other, and if settings were made on the middle of the image, the error in the glancing angle would amount to + 0.03 per cent., for  $\beta_0 = 2^\circ$  o' and  $\gamma = 15^\circ$ . Since 0.01 per cent. seems to be attainable, the angular subtense of the total length of the slit at the center of the crystal should not exceed 3° when very accurate data are sought experimentally.

TABLE II.

| <i>h</i> (mm.).* | ± a. |     | θ <sub>+</sub> .        |     |     | θ    |     |     |                     |
|------------------|------|-----|-------------------------|-----|-----|------|-----|-----|---------------------|
| 1.048156         | 15°  | 1'  | 10''                    | 30° | 2'  | 31″  | 0°  | 0′  | 11″                 |
| 1.049            | 14°  | 50' | $47^{\prime\prime}$     | 29° | 52' | 9″   | 0°  | 10' | 34''                |
| 1.050            | 14°  | 38' | 21″                     | 29° | 39' | 42'' | 0°  | 23' | 1″                  |
| 1.060            | 12°  | 22' | $4ar{4}^{\prime\prime}$ | 27° | 24' | 5''  | 2°  | 38' | 38''                |
| 1.070            | 9°   | 36' | 37″                     | 24° | 37' | 58'' | 5°  | 24' | $45^{\prime\prime}$ |
| 1.080            | 5°   | 37' | 37''                    | 20° | 38' | 59'' | 9°  | 23' | 44''                |
| 1.085            | 1°   | 10' | $43^{\prime\prime}$     | 16° | 12' | 4″   | 13° | 50' | 39′′                |
| 1.0852           | 0°   | 25' | 24''                    | 15° | 26' | 45'' | 14° | 35' | 57''                |

Table II. is intended primarily to illustrate the fact that, as the crystal is rotated, different points along the slit send rays through a given point on the focal circle. Since, in formula (18),  $\alpha$  is operated on by the cosine its sign cannot affect the values of the remaining quantities. In other words, two rays, having the same angular altitude  $\beta$ , can come from a given point of the slit and pass, after reflection, through a properly chosen, fixed point on the focal locus. The rays of such a pair have numerically equal values of  $\alpha$  but different arithmetical values of  $\theta$ , the position angle of the reflecting plane. As  $\beta$  changes sign so also will h do likewise [by (18)] so that two points on the slit and equidistant from the center of the same will simultaneously send two rays through the chosen focal point. Hence, for a given numerical value of  $\beta$ , four rays can diverge from the slit and, as the crystal is rotated, eventually converge to a single point on the focal circumference. It should be emphasized, however, that only finite segments of the slit can come into play in any actual case, since the angular positions of the reflector are theoretically limited by the condition that both the radiant point and the image point must lie on the same side of the crystal. (In

<sup>&</sup>lt;sup>1</sup> Units are given to fix the ideas. The angles only determine the *ratio*  $h/y_1$ .

general, the horizontal width of the crystal would restrict the length of the effective slit segment more than the formal limiting condition just mentioned.) If the rays be reversed, so as to treat the fixed point on the focal circle as source and the slit as an image locus, then the properties under discussion amount to a sort of astigmatism.

In Table II.,  $y_1 = 10$  cm.,  $x_2 = 5.00683$  cm.,  $y_2 = -8.65631$  cm.,  $\beta = 3^{\circ} 6' 21''$ ,  $\gamma = 15^{\circ} 0' 0''$ , and  $\eta = 30^{\circ} 2' 43''$ .

In applying photographic processes to the accurate determination of the glancing-angles (with respect to a definite kind of crystal) of characteristic X-rays it is not always convenient or desirable to place the plate either normal to the axis of the beam of rays or as a mean chord for a narrow region of wave-lengths. (Photographic films are unreliable for quantitative work.) Instead, the plate is placed normal to the line which passes through the center of the slit and intersects the axis of rotation at right angles. For sake of brevity, this line will be called the "collimation line." In this method care is usually taken to have the distance from the axis to the latent image equal to the distance from the slit to the axis, in order to take advantage of the uniplanar focal properties discussed above. For this case also, I have investigated, both analytically and arithmetically, the broadening of the photographic impressions due to the angular altitude  $\beta$ . Even when  $\alpha$  is kept equal to zero the datum finally required depends upon the solution of a cubic. It would be superfluous, therefore, to reproduce the analysis and numerical data in this place. Suffice it to state that, as might be expected, the displacement of the center of the image is greater here than in the hypothetical case of a cylindrical film previously treated. The relative increase in displacement is primarily due to the changing azimuthal obliquity of the rays with respect to the normal to the photographic plate. An approximate idea of the conditions prevailing in the present problem may be formed by referring to Fig. 4 and imagining the plate to be represented by a plane parallel to XOZ and passing through the point P, when  $\eta$  has its least value  $2\gamma$ . In all cases, the effect of  $\beta$  is to give too large a value for the apparent glancing-angle and hence to produce a positive error in the computed wave-length.

In all of the preceding cases the hypothesis was made that the reflecting planes were parallel to the axis of rotation. Even when the incident rays lie in the plane YOZ (Fig. 1) and are parallel to  $\overline{YO}$ , an effective obliquity is produced when the normal  $\overline{ON}$  describes, during the rotation of the crystal, a cone having  $O\overline{Z}$  as axis. As a consequence of the canting of the crystal the line on the spectrogram lacks parallelism to the central image formed by the undeviated rays. Even if it were possible

14

to measure the plate along the line in which it was intersected by the plane containing the collimation line and normal to the axis of rotation, the distance obtained would not be exactly correct, so that a slight error might be introduced in the calculated value of the glancing-angle.

The equation of the spectral line corresponding to the ideally simple conditions specified in the preceding paragraph will now be given without proof. It is

$$(\mathbf{I} - 2\cos^2\theta\cos^2\phi')x' - \cos\theta\sin 2\phi'\cdot z' + \sin 2\theta\cdot\cos^2\phi'\cdot y_0 = 0.$$
 (20)

The plane of the plate is expressed by  $y = -y_0$ . (Reference may be made to Fig. 1.) The origin of coördinates is taken on the collimation line. The axes of x' and z' lie in the plate and are parallel respectively to  $\overline{OX}$  and  $\overline{OZ}$ .  $\phi'$  denotes the angle which the normal  $\overline{ON}$  makes with its orthogonal projection on the plane XOY. It is counted positive when the complementary angle ZON is acute, that is, when the top of the crystal is tilted back from the axis of rotation.  $\theta$  symbolizes the angle which this projection makes with the axis  $\overline{OX}$ . Formula (20) may be freed from the auxiliary angle  $\theta$  by virtue of the relation

$$\sin \theta = \sin \gamma \sec \phi'.$$

The linear equation may be employed in two different ways. (a) By properly superposing two spectrograms, so as to magnify the angular error, an approximate value of the slope of the spectral line can be obtained. Equating the numerical value of this "slope" to its algebraic expression derived from (20), an estimate of  $\phi'$  may be gotten at once by solving the resulting quadratic in  $\cos 2\phi'$ . (b) The intercept on the axis of x', derived from formula (20), may be employed in calculating the order of magnitude of the error introduced by the maladjustment of the crystal.

Assuming  $y_1 = 10$  cm.,  $\gamma = 15^{\circ}$ , and  $\phi' = 1^{\circ}$ , the values of the remaining quantities were computed to be:  $x_0 = 5$  cm.,  $y_0 = 5\sqrt{3}$  cm.,  $\theta = 15^{\circ} \text{ o' } 8''$ , slope angle =  $92^{\circ} 13' 5\overline{1}''$ , and intercept on x' axis = 5.0027 cm. Therefore, the spectral image slants in the same general direction as the crystal face and makes an angle of  $2^{\circ} 13' 5\overline{1}''$  with the vertical. This angle exceeds  $2\phi'$  by 11.5 per cent. The linear displacement along the plate equals 0.027 mm. The calculated glancing-angle would be  $15^{\circ}$  o' 24'', which corresponds to an error of + 0.045 per cent. My short practical experience with the determination of glancing-angles leads me to believe that, in the vicinity of  $15^{\circ}$ , it is possible to attain an appreciably higher degree of accuracy than 1/22 per cent.

Practical Deductions.-In the first place, the preceding discussion of

#### HORACE SCUDDER UHLER.

the asymmetric broadening of spectral images due to obliquity in angular altitude leads to the conclusion that, when the highest attainable accuracy is required, diaphragms should be used so as to limit the vertical height of the incident beam of X-rays. Probably the most advantageous location of one of the diaphragms would be (in the case of primary rays) on the side of the anticathode itself. Although all the cases treated analytically involved the assumption that the slits were of zero width, it seems obvious that the various errors will not be decreased when the slits have the finite horizontal aperture necessary for the practical transmission of energy. In the following paragraphs, therefore, the hypothesis will be made that the rays do not depart appreciably from planes perpendicular to the axis of rotation.

In the usual photographic method of determining glancing-angles it is necessary to measure the perpendicular distance from the axis of rotation to the plate. It is very difficult, if not impossible, so to adjust the apparatus as to satisfy the definition of this distance, for, in the case of rays of sensible penetration, the *mean* effective reflecting plane, which should contain the axis of rotation, lies at a depth from the front face of the crystal that involves uncertainty. Even if the crystal were in perfect adjustment for one particular wave-length it would not remain so for rays of appreciably different penetration. Doubt also arises as to whether the gelatin side of the plate always clamps at the same distance from the axis of rotation, no matter how rigid the plate-holder itself may be. (Gelatin is compressible, commercial dry plates are very often curved and twisted, etc.)

The errors arising from these, and from many other, causes may be largely, if not entirely, eliminated by the "Method of Displacement." As far as I can find from the literature of the subject this simple idea is new. It consists in taking one exposure when the plate is at a certain distance from the crystal and then a second exposure when it is at a different distance from the reflector. The displacement of the spectral image, corresponding to some one wave-length, is a function of the distance through which the plate has been translated parallel to the collimation line. The form of the function and the details of the calculation of the glancing-angle depend respectively upon the value of the constant angle between the normal to the plate and the collimation line, and upon whether the measurements are absolute or are based upon adjacent images pertaining to known wave-lengths. The interval of translation may be determined with ease and great accuracy, whereas only an approximate value of the distance between the plate and the axis of rotation is required in any case. The plate can be pressed sufficiently flat by strong springs and, as it cannot move relative to its holder, no doubt can arise concerning the distance through which the plate has been translated. On the other hand, the method of displacement involves the fundamental assumption that the images of the same spectral line are sensibly identical in the two positions of the plateholder. As far as I have been able to find, both theoretically and experimentally, this assumption is fulfilled by using *two narrow slits of exactly the same width*. (Obviously, both slits must be completely filled by the beam of X-rays.)

The formation of a beam of X-rays of constant cross-section, by two slits of identical opening, will now be explained. As stated before, it will be assumed that diaphragms have been interposed in the path of the beam in such a manner as practically to eliminate any asymmetric broadening of the images due to the angular altitude  $\beta$ . For the time being, the hypotheses will also be made that there is no penetration and that the reflecting plane contains the axis of rotation. On the contrary, the assumption that the slits are of zero width will no longer be retained.

The plane of the diagram (Fig. 5) is taken normal to the mutually



parallel long-axes of the slits  $S_1$  and  $S_2$ , but it does not have to contain the collimation line. Now, by the fundamental theorem of the focal circle (or cylinder), any ray which passes through the incidence edge  $E_1$ of slit  $S_1$  will, after reflection from the crystal at the given glancingangle  $\gamma$  (monochromatic radiation being assumed), pass through the point  $I_1$ . The point  $I_1$  is at the same distance from the axis of rotation Oas the point  $E_1$ , and the deviation of the line  $\overline{OI}_1$  with respect to the line  $\overline{E_1O}$  equals  $2\gamma$ . The ray in question is not required to strike the crystal at the point O. If the ray also passes through the emergence

Vol. XI. No. 1. HORACE SCUDDER UHLER.

edge  $E_2'$  of slit  $S_2$  it will, after reflection, pass through a point  $I_2'$ . This point is likewise determined by the conditions  $OI_2' = E_2'O$  and  $\angle E_2'OI_2'$  $= \pi - 2\gamma$ . Hence, one extreme diagonal ray  $\overline{E_1E_2}$  takes the direction  $I_2'I_1$  after reflection. Similarly the incident rays  $E_1'E_2$ ,  $E_1E_2$ , and  $E_1'E_2'$  will become the reflected rays  $I_2I_1'$ ,  $I_2I_1$ , and  $I_2'I_1'$ , respectively. In general, therefore, a ray which passes through any point P within the rectangle  $E_1E_2E_2'E_1'$  will, after selective reflection, pass through the homologous image point P', such that  $\overline{OP'} = \overline{PO}$  and  $\angle POP' = \pi - 2\gamma$ . Since all rays that pass between the jaws of both slits are confined between the parallel segments  $E_1E_2$  and  $E_1'E_2'$  it follows at once that the reflected beam cannot escape through the sides  $I_2I_1$  and  $I_2'I_1'$  of the rectangle  $I_1I_2I_2'I_1'$ . Consequently as long as the gelatin side of a plate is moved parallel to itself (along the collimation line or in some other direction), and is kept within the limits set by the condition that the sensitized surface shall not intersect the reflected beam at any point outside of the rectangle  $I_1I_2I_2'I_1'$ , the images will be of constant width, and their relative shifts will be directly proportional to the displacement of the plate. As the length of the rectangle  $I_2I_1$  is equal to the constant distance  $E_1E_2$  between the slits it is independent of the glancing-angle involved. Hence, the length  $I_2I_1$  is dependent neither upon the wavelength of the X-rays nor upon the grating-space of the crystal. On the contrary, the projection of  $I_2I_1$  on the collimation line is a function of the glancing-angle. In particular, if the photographic plate is kept normal to this line the interval of translation is a little less than  $I_2I_1 \cos 2\gamma$ .

If all the incident rays were strictly parallel to  $E_1E_2$  then all of the reflected rays would be exactly parallel to  $I_2I_1$ , the beam would experience reflection for only one angular position of the crystal (assuming that the curve of reflection is extremely steep on both sides of the maximum), and nothing would be gained by rotating the crystal. These conditions would be fulfilled quite independently of penetration and of any eccentricity of the mean effective reflecting plane. By drawing lines, representing traces of planes, parallel to the lines which pass through O (Fig. 5) and which indicate three positions of the single noneccentric reflecting plane, it is easy to see that the effects of symmetrical penetration and of eccentricity would be respectively to increase the cross-sections  $I_1I_1'$  and  $I_2I_2'$ , and to shift the principal axis of the reflected beam parallel to itself. [The rays  $\overline{IR}$  and  $\overline{I'R'}$  (Fig. 3) are parallel and arise from the single incident ray SII'.] Simple displacement without alteration either in direction or in constancy of cross-section would have no influence on the present method of determining glancing-angles. Hence, all restricting conditions, save  $\beta$  negligible, have been removed.

18

### SECOND

The method has been tested experimentally, by Dr. C. D. Cooksey<sup>1</sup> and myself, for the fairly soft rays of the K series of gallium and of the L series of tungsten, and found to be very convenient and accurate. We have not had time, as yet, to try it with very penetrating X-rays. If, for some unforeseen reason, the scheme of using two equal slits simultaneously should eventually be found unsatisfactory for very hard rays, the method of displacement may still be applied by using slit  $S_1$  alone when the plate is near the focal spot  $I_1I_1'$ , and then employing slit  $S_2$ alone with the plate near  $I_2I_2'$ . The last application of the general method might require especially accurate construction and adjustment of the spectrograph, but it would retain all the desirable features (such as intensity) of the usual method of experimentation together with the great advantage of knowing precisely how far the plate has been translated.

#### SUMMARY.

1. The general equations of incident and reflected rays have been derived.

2. It has been demonstrated that, in general, not more than two rays are determined by one point on the incident segment, one point on the reflected segment, and the glancing-angle.

3. The special theorem of the focal circle has been stated and proved in a perfectly general manner. It has been shown that this theorem involves the following assumptions: (a) The rays of a pencil must all lie in one plane perpendicular to the axis of rotation of the crystal, (b) the rays must not penetrate the crystal to a finite depth, (c) the reflecting plane must contain the axis of rotation, and (d) the slit must act as a mathematical line source.

4. It has been shown analytically that a circular envelope arises when the reflecting plane is parallel to the axis of rotation, but does not contain this axis. Special properties of this locus have been demonstrated.

5. It has been proved that rays having finite angular altitude produce asymmetric broadening of the spectral images even when the azimuth is zero. It has been shown that, when the angular altitude is constant and the azimuth is finite and variable, the bundles of rays have astigmatic properties. The fact that this broadening is always in such a direction as to lead to too large a value of the glancing-angle has been demonstrated. The special case of a photographic plate normal to the line of collimation has been discussed.

6. The results obtained from an analytical study of the alteration in

<sup>1</sup>See "The K Series of the X-Ray Spectrum of Gallium," by H. S. Uhler and C. D. Cooksey, PHY. REV., N.S., p. 645, vol. X., Dec., 1917.

the slope and intercepts of a spectral line, due to tilting the reflecting planes of atoms with respect to the axis of rotation, have been given.

7. Whenever possible, the practical bearing of the theoretical considerations has been discussed. In particular, the theoretical and experimental aspects of a supposedly new method for the accurate determination of glancing-angles have been presented at some length. In so doing, slits of *finite* width and rays of sensible penetration have been considered. The general method involved has been styled the "Method of Displacement," and two ways of applying it have been suggested. One of these ways has been tested experimentally and found very convenient and accurate.

SLOANE PHYSICAL LABORATORY, YALE UNIVERSITY, August 17, 1917.