

# GEOMETRY OF THE TWO-CRYSTAL X-RAY SPECTROMETER<sup>1</sup>

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In order to avoid rather considerable gearing linkages the two-crystal spectrometer (Compton and Allison, 1934) is often arranged so that the x-ray tube, one of the crystals and the detector remain fixed while the other crystal is rotated through a small angle to scan the spectral region under study. The limitation on the spectral region which can be scanned at one such setting is imposed by the size of the crystals and of the detector opening. As either the first or the second crystal is rotated the region of Bragg reflection moves across the crystal surface. As shown later on, this "walking" turns out to be considerably larger when the first of the two crystals is rotated.

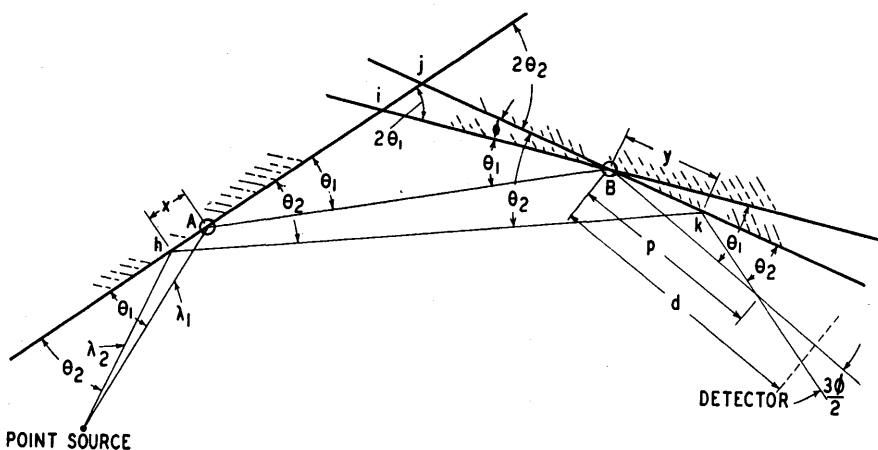


Figure 1. Rotation of *second* crystal. Ray paths through the two-crystal spectrometer for wavelengths  $\lambda_1$  and  $\lambda_2$ ; ( $\lambda_2 > \lambda_1$ );  $A$  and  $B$  are fixed axes of rotation of the first and second crystals respectively.

In figure 1 are shown two crystals whose reflecting faces are perpendicular to the page and whose fixed axes of rotation are at  $A$  and  $B$ . The ray  $\lambda_1$  is reflected at Bragg angle  $\theta_1$  while the ray  $\lambda_2$  of somewhat longer wavelength is reflected at Bragg angle  $\theta_2$  after rotation of the *second* crystal through a small angle  $\phi$  while the first crystal remains fixed. It is clear that the second ray will be reflected from points  $h$  and  $k$  different from  $A$  and  $B$ . It is the purpose of this paper to investigate the walking of the central ray as either the first or second crystal is rotated. The discussion is limited to central rays.

Simple geometrical considerations of figure 1 show that

$$\theta_2 = \theta_1 + \phi/2$$

$Ah = x = L \frac{\sin \phi/2}{\sin (\theta_1 + \phi/2)}$ , where  $L$  is the distance from the source to the first axis  $A$ ; and

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$$y = Bk = x + \frac{S}{2 \cos \Theta_1} \left[ 1 - \frac{\sin 2\Theta_1 - \sin \phi}{\sin (2\Theta_1 + \phi)} \right], \text{ where } S \text{ is the separation}$$

between the axes,  $A$  and  $B$ . If we define  $p$  to be the distance from the second axis  $B$  to the intersection of the rays, then

$$p = y \frac{\sin (\Theta_1 + \phi/2)}{\sin 3\phi/2}.$$

When a detector is located at a distance  $d$  from the second axis, the walking,  $w$ , of the beam on the detector is given by

$$w = (D-p) \sin 3\phi/2, \text{ or } w = y \sin (\Theta_1 + \phi/2) - D \sin 3\phi/2.$$

Table 1 shows representative values for the walking for three values of  $\Theta_1$  and four values of  $\phi/2$ . The values of  $L$ ,  $S$  and  $D$  were chosen as being fairly typical. The walking on the crystals is seen to be independent of crystal parameters and of x-ray wavelength, depending only on the Bragg angle and the dimensions of the spectrometer.

TABLE 1

*Distances in Inches ( $L=12$  in.;  $S=8$  in.;  $D=4$  in.)*

$\Theta_1$	$\frac{\phi}{2} (= \Delta\Theta)$	x	y	w
5°	15'	.572	.954	.035
	30'	1.093	1.821	.070
	1°	2.003	3.339	.140
	1°30'	2.775	4.629	.210
30°	15'	.104	.173	.035
	30'	.206	.344	.070
	1°	.407	.678	.140
	1°30'	.601	1.002	.210
50°	15'	.068	.113	.035
	30'	.136	.226	.070
	1°	.269	.449	.140
	1°30'	.401	.669	.210

At Bragg angles greater than 30° and less than 75° and for  $\Delta\Theta \leq 1^\circ 30'$  the following simple linear formulas can be used with an error of less than 5 percent.

$$\begin{aligned} x &= L (\phi/2) \csc \Theta_1 \\ y &= (L + 1.05 S) (\phi/2) \csc \Theta_1 \\ w &= (\phi/2) (L + 1.05 S - 3D). \end{aligned}$$

Figure 2 shows the geometry when the first crystal is rotated.  $\Theta_1$ ,  $\Theta_2$  and  $\phi$  are defined as before. It follows that

$$\begin{aligned} \Theta_2 &= \theta_1 - \phi/2 \\ Ah = x &= L \frac{\sin 3\phi/2}{\sin (\Theta_1 - \phi/2)} \\ Bk = y = x - S &= \left[ \frac{\sin \Theta_1 - \sin (\Theta_1 - \phi)}{\sin (2\Theta_1 + \phi)} \right] \end{aligned}$$

$$\text{and } p = y \frac{\sin \Theta_1}{\sin \phi/2}.$$

The walking across the detector is given by

$$\begin{aligned} w &= (D-p) \sin \phi/2, \text{ or} \\ w &= y \sin \Theta_1 - D \sin \phi/2 \end{aligned}$$

Table 2 shows representative values for the walking. The same values of  $L$ ,  $S$  and  $D$  were used.

An approximate formula useful as before for Bragg angles between  $30^\circ$  and  $75^\circ$  and for small  $\Delta\theta$  is

$$x = 3 L \csc \theta_1 (\phi/2)$$

For this case, no simple approximations to  $y$  and  $w$  similar to those of the first case are possible.

TABLE 2  
Distances in Inches ( $L=12$  in.;  $S=8$  in.;  $D=4$  in.)

$\theta_1$	$\frac{\phi}{2} (= \Delta\theta)$	$x$	$y$	$w$
$5^\circ$	15'	1.897	1.515	.115
	30'	4.004	3.274	.250
	1°	9.003	7.663	.598
	1°30'	15.422	13.563	1.077
$30^\circ$	15'	.316	.197	.081
	30'	.638	.402	.166
	1°	1.296	.835	.348
	1°30'	1.973	1.297	.544
$50^\circ$	15'	.206	.148	.096
	30'	.413	.297	.193
	1°	.832	.600	.390
	1°30'	1.257	.910	.592

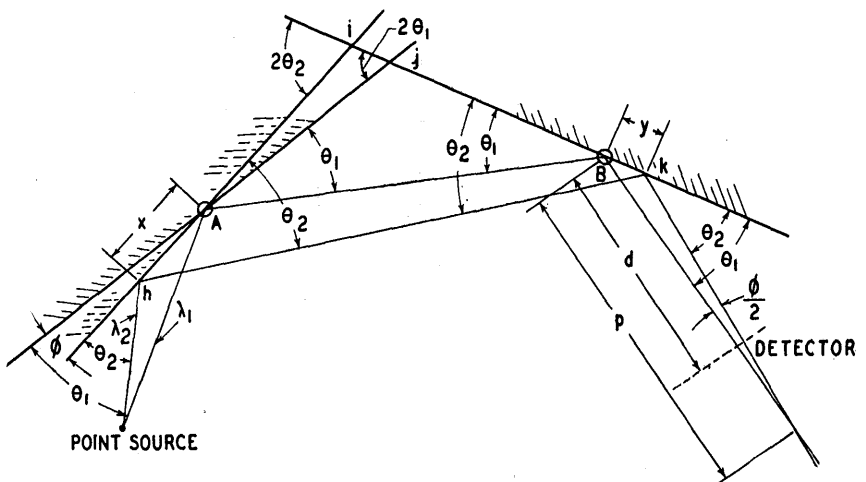


Figure 2. Rotation of first crystal. Ray paths through the two-crystal spectrometer for wavelengths  $\lambda_1$  and  $\lambda_2$ ; ( $\lambda_2 > \lambda_1$ );  $A$  and  $B$  are fixed axes of rotation of the first and second crystals respectively.

#### REFERENCES

- Compton, A. H., and S. K. Allison. 1934. X-Rays in Theory and Experiment. D. Van Nostrand Co., New York. p. 709.