Physical Chemistry

**Measuring a Lattice Constant from the Diffraction Pattern**

Virginia B. Pett
The College of Wooster

Consider a light shining through a diffraction grating, producing alternating bright and dark bands on a screen. The constructive interference that gives rise to a maximum in light intensity is illustrated in Figure 1. For constructive interference, the distance C in Figure 1 must be equal to an integer number of whole wavelengths.

$$C = n\lambda \qquad (1)$$

where $n$ is an integer and $\lambda$ is the wavelength of the light. For the first intensity maximum,

$$C = \lambda \qquad (2)$$

The distance, C, is related to the angle Ø and the grating width, $r$, by eq. 3.

$$C = r \sin Ø \qquad (3)$$

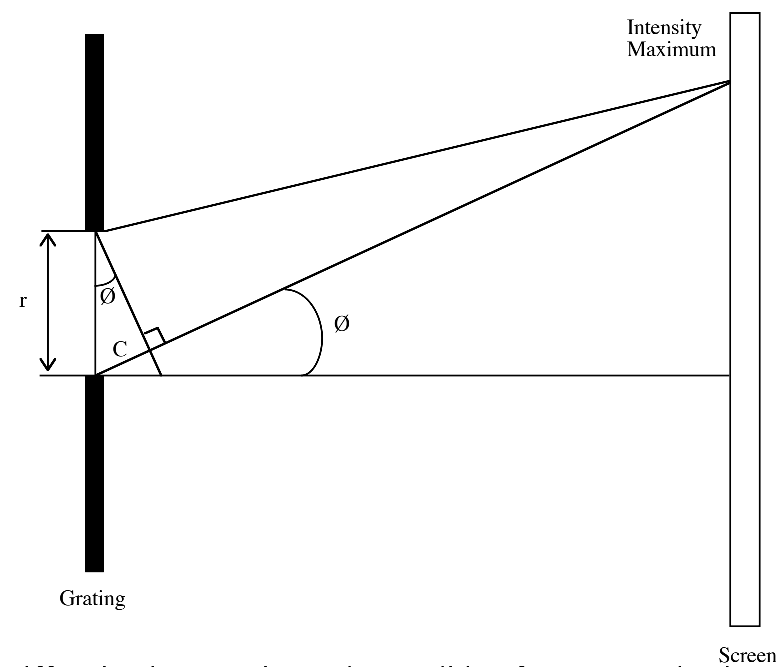


Figure 1. Diffraction by a grating. The condition for constructive interference and diffraction maxima is given in eq 1.

If instead of a diffraction grating we have a single crystal aligned so that a direct axis coincides with the rotation axis, planes in the crystal—like the lines on a diffraction grating—diffract the light. In this case the planes in the crystal are very close together, and we need to use light with very short wavelength, on the order of Ångströms. We see the diffraction maxima on the X-ray detector or film as rows of dark spots, and we can measure the distance along the film from the direct X-ray beam to the various maxima. The same condition holds, that the distance C must be equal to an integer number of wavelengths for constructive interference to occur.

The relationship between the angle Ø and the experimentally measured distances $Y_n$ on the X-ray detector or film is shown in Figure 2 and in eq 4; $R$ is the distance between the crystal and detector.

$$\tan \text{Ø} = \frac{Y_n}{R} \tag{4}$$

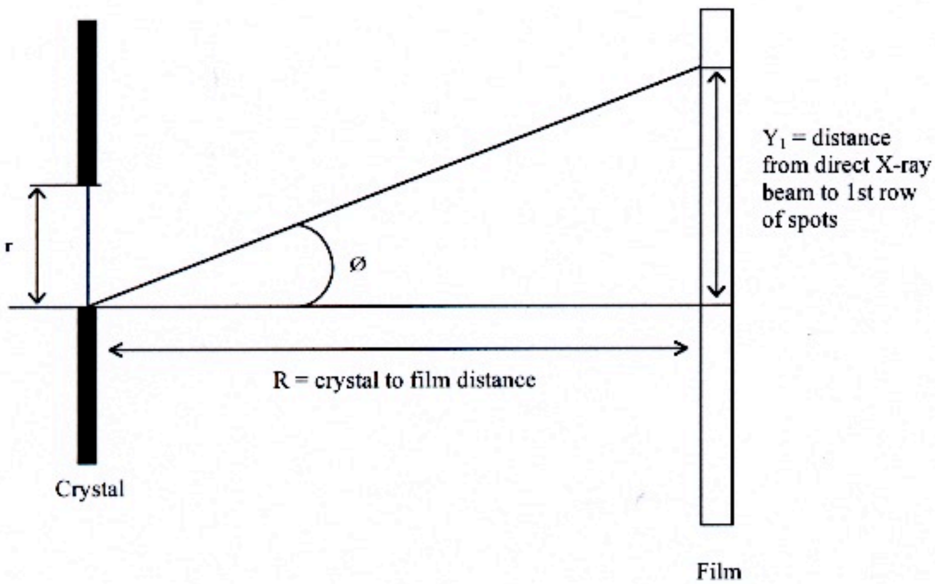


Figure 2. Experimentally measured distances $Y_n$ for diffraction by a crystal with lattice constant $r$, placed at a distance $R$ from the detector.

Combining equations 1, 3, and 4 gives an expression for the length of one side of the unit cell, $r$, in terms of the measurable distances on the detector or film $Y_n$ and the crystal to detector distance $R$.[1] (For the Weissenberg camera, $R$ is the radius of the film cassette, usually 28.65 mm and $\lambda$ = 1.5418 Å for Cu $K_\alpha$ radiation.)

$$C = n\lambda = r \sin\left[\arctan \frac{Y_n}{R}\right] \tag{5}$$

or rearranging:

$$r = \frac{n\lambda}{\sin\left[\arctan \frac{Y_n}{R}\right]} \tag{6}$$

The cell constant can be more accurately determined by measuring $Y_n$ for several values of $n$. If we plot $n$ vs. $\dfrac{\sin[\arctan \frac{Y_n}{R}]}{\lambda}$, a straight line is obtained with slope r and zero intercept.

[1] Equations 5 and 6 are not correct if $r$ is an inclined axis. See Stout, G.H. & Jensen, L.H. (1989). *X-Ray Structure Determination: A Practical Guide*, 2nd ed. New York: John Wiley & Sons, pp 104–106.