Laboratory Notes

and the second scan parallel but at a known distance (for example \( h = 0.2'' \)) from the first one. This double scan method has many advantages:

(a) Since the two scans will intercept many ‘circles’ in 4 points, one can deduce the exact position (in both \( x \) and \( y \) directions, \( x \) direction being the direction of the scans) of their centers which are the two poles of the diffraction pattern (at 0 and 180°). This determination will help to give a better estimate of the \( d \) spacing of each line.

(b) By requiring that a real line must show up on both scans at the same distance from one of the poles, one will eliminate the spurious lines due to dust or noises on the film.

(c) Since many estimates of the integrated intensity and of the \( d \) spacing for each line can be obtained, the average results are better than with only one scan.

A FORTRAN program (named POWDR) has been written to analyze automatically the data from a double scan of any powder photograph. The results from a double scan of a powder film taken with a quartz sample (\( \text{SiO}_2 \)) show very good agreement with the X-ray powder data file.

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Attachment for motorized rotation about the polar axis of a goniostat.

Motorized rotation of the crystal at a uniform rate about the diffraction vector is essential for the experimental investigation of X-ray multiple diffraction effects and may be required also for the investigation of anisotropic extinction effects or of absorption in irregularly-shaped crystals. The quarter-circle goniostat of the General Electric single crystal orieniter (Furnas, 1966) has no provision for motorized rotation of the specimen crystal about the polar (\( \varphi \)) axis of the goniometer head. To rotate the crystal about the diffraction vector of a specified X-ray reflexion (azimuthal scan), one adjusts the arcs of the goniometer head until the reflexion occurs at the setting \( \chi = 90^\circ \), where \( \chi \) is the inclination angle of the polar axis from the vertical. The diffraction vector is then parallel to the \( \varphi \) axis, and rotation about this axis alone does not violate the Laue conditions on the chosen reflexion. The attachment we describe here facilitates such rotation, at the convenient rates of either 0-2 or 5\(^\circ\). min\(^{-1}\).

The device consists of a mains-operated synchronous motor (Venner) mounted on a dovetail bracket, and a shaft to which are attached four interlocking gears. It is shown in operation, with the goniostat at the \( \chi = 90^\circ \) setting.

in Fig. 1. The dovetail bracket bearing the motor has been mated to the curved dovetail track of the goniostat and locked in position by means of a screw-operated wedge clamp so that the distance from the spindle of the motor to the \( \varphi \) axis drive spindle is equal to the length of the shaft. The drum which normally attaches to this \( \varphi \) spindle (and by means of which manual rotation about the \( \varphi \) axis is achieved) has been removed, and the lower end of the shaft and the largest gear have been fastened to the spindle of the motor. One revolution of the \( \varphi \) spindle produces a rotation of 2\(^\circ\) about the \( \varphi \) axis. The spindle of the motor rotates at 30 revolutions per hour and the gears reduce this by 5:1. Hence, in the mode of operation shown in Fig. 1, the attachment causes the crystal to rotate about the \( \varphi \) axis at the rate of 0-2\(^\circ\). min\(^{-1}\). Rotation at the rate of 5\(^\circ\). min\(^{-1}\) is attained simply by inverting the shaft.

Fig. 1. The attachment in operation on the goniostat.

Fig. 2. Chart recording of complete azimuthal scan about the 222 diffraction vector of silicon (Cu \( K\alpha \) radiation).

Fig. 2 shows a complete (360\(^\circ\)) azimuthal scan at the rate of 5\(^\circ\). min\(^{-1}\) about the diffraction vector of the ‘forbidden’ 222 reflexion in silicon, obtained with copper \( K\alpha \) radiation diffracted by a ground spherical crystal. The base intensity is due to the 222 primary reflexion, while the peaks (equivalent peaks occur every 30\(^\circ\)) are perturbations due to the simultaneous excitation of additional reflexions.

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Reference


A double-scan method for powder X-ray diffraction film.

There exist commercial devices that can scan a powder X-ray diffraction film and enregister the optical density measurements on a digital magnetic tape. Using this data on a computer, one hopes to be able to estimate automatically the intensity and \( d \) spacing of all the lines on the film. Unfortunately this computer program is almost impossible to write since it is difficult to distinguish real but weak lines from dust or noise on the film. In order to make an automatic analysis of powder film possible, we suggest that it be scanned twice, the first scan near the center of the diffraction pattern,