

(vii) radiation damage in single crystals; and (viii) influence of the Borrmann effect on diffraction images of dislocations (A. R. Lang, in preparation).

Fig. 2 shows a projection topograph of dislocations in a  $\{111\}$  slice of silicon, taken with a 220 reflection from planes normal to the slice. The area covered is about  $5 \text{ mm.} \times 4\frac{1}{2} \text{ mm.}$  Pendellösung fringes may be seen in the bevelled edge of the slice. Noteworthy is the strong visibility of dislocations whose Buerger's vector is normal to the reflecting planes.

*Acta Cryst.* (1959). **12**, 250

**Determination of lattice parameters directly from Bunn charts.** By P. P. WILLIAMS, *Dominion Laboratory, Wellington, New Zealand*

(Received 2 December 1958)

Although the Bunn (1945) charts for indexing X-ray powder diffraction patterns of tetragonal and hexagonal structures are easier to use than the Bjurstrom (1931) charts, they suffer from the disadvantage that in plotting values of  $1/d^2$  (or  $\sin^2 \theta$ ) on a logarithmic scale, knowledge of the actual dimensions of the unit cell is lost, and only the shape of the cell can be deduced directly from the plot. It is often convenient to have a means of checking calculations of axial lengths from indexed lines, and to have the means of deducing rapidly the diffraction pattern that will be produced by a structure with given axial lengths. A simple addition to the Bunn chart allows this to be done.

The Bunn chart is constructed on logarithmic scales, and is used by plotting  $\log \sin^2 \theta$  for lines on the diffraction pattern on a strip of paper, using the same scale as the ordinate of the chart. The strip is moved about on the chart until a good match is obtained between positions of  $\sin^2 \theta$  and curves on the chart. If in addition to the values of  $\sin^2 \theta$  for the diffraction maxima, a reference mark at a fixed value of  $\sin^2 \theta$  is also placed on the strip, information not only about the relative

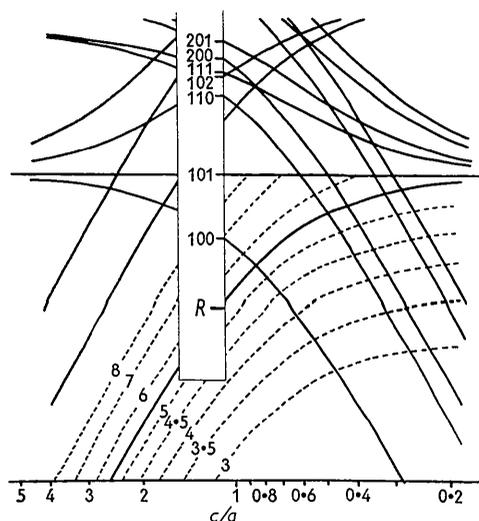


Fig. 1. The Bunn chart for hexagonal structures, with  $c$  axial lengths loci marked.

The strip bears the pattern of  $\alpha$ -quartz, and a reference mark  $R$ , at  $\sin^2 \theta = 0.02$ .

This work was made possible by a grant from the National Science Foundation, receipt of which is gratefully acknowledged.

### References

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positions of the diffraction lines but also about their actual positions is retained on the strip. At a matching position of the strip, the position on the chart of the reference mark can be correlated with an axial dimension.

At a series of matching positions of the strip, for patterns of structures with one axial length (say the  $c$  axis) fixed, and varying axial ratios, the locus of the reference mark is clearly a curve whose vertical distance from the 001 curve on the chart is constant. The distance of the locus from the 001 curve can be calculated, but it is more easily plotted semi-empirically. On a strip of paper is plotted the reference mark to be used, and values of  $\sin^2 \theta$  corresponding to the 001 spacing for a selection of values of  $c$ , at the wavelength to be used. Then the strip is placed vertically on the chart, and the loci of the reference mark plotted as the strip is moved about, keeping each of the  $\sin^2 \theta$  marks in turn on the 001 curve. Fig. 1 shows the lower part of a Bunn chart for hexagonal structures with the axial-length loci plotted for  $c$  axes of 3 Å to 8 Å, for use with a reference mark at  $\sin^2 \theta = 0.02$  and  $\text{Cu } K\alpha$  radiation. Interpolation between the curves is carried out logarithmically along the ordinate. The strip bears the first few lines of the  $\alpha$ -quartz pattern, matched with curves on the chart. The position of the reference mark in relation to the  $c$  axial length loci shows the  $c$  axis to be 5.43 Å, and the axial ratio,  $c/a$ , is read off as usual as 1.10, from which the  $a$  axis is calculated as 4.95 Å. Refinement of these axial lengths by considering high-angle lines gives  $c = 5.405$  Å and  $a = 4.913$  Å (Swanson & Fuyat, 1953).

The process can be reversed to predict the pattern that a specific structure will produce, by placing a strip of logarithmically calibrated paper on the chart so that the reference-mark position falls at the point on the chart defined by the length of the  $c$  axis and the axial ratio. The values of  $\sin^2 \theta$  at which lines may appear can then be read directly off the strip at the intersections of the edge of the strip with curves on the chart.

### References

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