

cylinder radius, R , because of the positive and negative values possible for the c_k parameters of structure. In the compound cylinder case, when k (or the product $k\sigma_b$) is sufficiently large R_k'' approaches R_0 , in which case individual filaments are essentially diffracting independently. One must keep in mind, however, that as $k\sigma_b$ approaches zero, leading essentially back to the smooth cylinder case, R_k'' should approach the relatively large value R but not become infinitely large as given by the equation. This difficulty is a result of an excessive upper limit (∞) assigned during a radial integration in the evaluation of $|F_{kr}''|^2$ but is easily avoided in practical cases by restricting application to layer lines of high index.

R_k can be used generally wherever R occurs in the theory for the particular case of the smooth cylinder, with restriction required, however, to applications involving reciprocal-array disk shapes and dimensions. For example, disk diameters are generally calculable from $\{2\sqrt{(-\ln 0.5)/\pi\bar{\nu}R_k}\}$, which was derived above only for the smooth cylinder. On the other hand, R_k substituted for R everywhere in equation (1) does not lead to appropriate approximations of equations (3) and (5).

In actual studies one obtains experimental shape functions for a given specimen as follows: A given point of the k th disk is brought into the plane of reflection by a tilt θ to a position whose co-ordinates in the reflection plane are ξ and ζ_k . As is apparent from Fig. 1,

$$\zeta_k = y_k^* / \cos \theta.$$

Also $y_k^{*2} + r^{*2} = \xi^2 + \zeta_k^2$, from which it follows, since $y_k^* = k\lambda/b_0$, that

$$r^* = \sqrt{\{\xi^2 + (k\lambda/b_0)^2 \tan^2 \theta\}}.$$

When this value of r^* is used in equation (7), one obtains the expression (useful under pinhole-camera conditions) indicating the way in which at a given tilt, θ ,

intensity should vary along the k th layer line as a function of ξ , the angular departure from the meridional line. On the other hand, one may examine how intensity at constant ξ on a given line depends upon tilt. The former application deals with 'line shape', the latter with 'persistence of intensity with tilt'. This program is an ideal one; actual methods will be detailed elsewhere in connection with a presentation of results of collagen studies.

As illustration of phenomena to be expected of the three types of diffractor under consideration, Fig. 2 indicates diagrammatically the diffraction patterns expected of them under the condition of zero tilt. Only relative line lengths, corresponding to intersections of disk diameters with the reflection plane, are shown. The distinctively different characters of these patterns suggest that the models should be readily recognizable when encountered. In actual cases one sometimes finds combinations of these diffraction effects, but study of the observed line lengths (and similar quantities) in relation to these simple theoretical cases can suggest means for arriving at a model tailored to fit the diffractor at hand.

References

- BEAR, R. S. & BOLDUAN, O. E. A. (1950). *Acta Cryst.* **3**, 230.
 BOLDUAN, O. E. A. & BEAR, R. S. (1950). *J. Polym. Sci.* (in press).
 JAMES, R. W. (1948). *The Optical Principles of the Diffraction of X-Rays*. London: Bell.
 MACGILLAVRY, C. H. & BRUINS, E. M. (1948). *Acta Cryst.* **1**, 156.
 SCHMITT, F. O. & GROSS, J. (1948). *J. Amer. Leath. Chem. Ass.* **43**, 658.
 WATSON, G. N. (1944). *Theory of Bessel Functions*. Cambridge: University Press.
 WRINCH, D. (1946). *Fourier Transforms and Structure Factors*. Cambridge, Mass: Murray.

Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

Acta Cryst. (1950). **3**, 241

The diffuse scattering of NaClO₃. By M. S. AHMED and K. LONSDALE, *Chemistry Department, University College, Gower Street, London W.C. 1, England.*

(Received 3 November 1949)

In a recent paper (Garrido, 1948*a*; published in full in the *Memorias de la Real Academia de ciencias exactas de Madrid* (Garrido, 1948*b*)) the diffuse scattering regions surrounding the reciprocal-lattice points of NaClO₃ are deduced from a series of Laue photographs, and are alleged to show long protuberances along two cube-axis directions, resulting in a square cross.

Sen (1949) has pointed out that these results conflict with calculations from the thermal vibration theory, and infers that the theory is thereby disproved.

Ramachandran & Wooster (1950) have, however, repeated the measurements of diffuse scattering, for selected sections of reciprocal space, using the Geiger-counter method and very perfect NaClO₃ crystals; and

they find complete agreement between their observations and calculations from the Jahn formula. Thus the thermal-vibration theory is confirmed, but the question still remains as to why the photographic method did not give the same result.

Why, in fact, did Garrido find regions shaped like a square cross instead of like a circular bun with a slightly depressed middle? Could it have been disorder or distortion in his crystals, or is the photographic method unreliable?

One of us (M.S.A.) has repeated some of Garrido's photographic observations and has also taken some other photographs. Those taken in the same crystal orientation (but with filtered Mo $K\alpha$ radiations, so that the photographs are much clearer) give pictures exactly like those published, with interpretative diagrams, in the Madrid paper. But we disagree with Garrido's deductions from them, for the following reasons:

(1) Garrido's photographs were taken in various crystal orientations relative to the incident X-ray beam, but in every case with the [100] axis vertical. The (100) plane is therefore horizontal and parallel to the X-ray beam, but the sphere of reflexion cuts the diffuse 200 domain, so that the $D200$ reflexion always appears, and it is found to be unchanged for different crystal settings. Now these observations show that the 200 diffuse-scattering domain is shaped like a circular bun, perpendicular to the [100] reciprocal-lattice vector (Fig. 1(a)). If it had been shaped like a cross, as Garrido suggested, the $D200$ spot would have been doubled in orientations where the X-ray beam is nearly along $\langle 011 \rangle$ (Fig. 1(b)). This is not the case (cf. Fig. 32 of the Madrid paper, Laue diagram 595, Plate VI, taken with the X-ray beam at $48^\circ 30'$ from the cube axis).

(2) A further independent test of this point could have been made by taking photographs with the [110] axis (or any diagonal direction) vertical. If the shape of the regions had been that given by Garrido, such photographs would have shown a doubling of all diffuse spots (Fig. 1(c)). Since the shape is in fact that of a circular bun, the diffuse spots are unchanged in appearance whatever axis in the 001 reciprocal net is vertical.

(3) A further test of the proposed domains may be made by examining the height of the diffuse spot. (In the case of 020 (Figs. 36 and 37, Madrid paper), this would be its dimension parallel to [100], the axis about which the crystal was being rotated.) If the shape of the domain had been cruciform, the 020 diffuse spot would have been oval

or circular and of constant intensity at the perimeter until the Bragg reflecting position was nearly reached, when there would have been an abrupt elongation (still with constant intensity at the perimeter) to a shape about eight times the original height, but of the same width. The result would have been a marked *streaking* in these positions only; such a streaking does not occur, for this or any other reflexion.

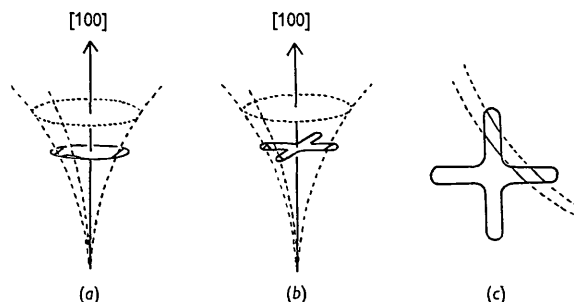


Fig. 1. (a) When the 100 domain is circular, the $D200$ reflexion is unchanged as the sphere of reflexion moves round. (b) When the 100 domain is cruciform, the $D200$ reflexion should sometimes be doubled, sometimes single. (c) A doubling of the diffuse reflexions is also to be expected when a diagonal axis is vertical.

We find, in fact, that both Garrido's photographs and ours lead to the shape of the diffuse scattering regions predicted by the Jahn formula, using the latest values of the elastic constants (Lonsdale, 1948). This conclusion has now been accepted by Dr Garrido (private communication). It is not necessary to use exceptionally good crystals for the photographic method; it is far more important to clear the background of the photographs from fog, due to air scattering of short wave-lengths and other extraneous effects, so that the exact shape, extent and intensity of the diffuse scattering due to the $K\alpha$ radiation only can be clearly distinguished.

References

- GARRIDO, J. (1948a). *Acta Cryst.* **1**, 3.
 GARRIDO, J. (1948b). *Mem. R. Acad. Madr. Serie físicas*, **2**, no. 4.
 LONSDALE, K. (1948). *Acta Cryst.* **1**, 142.
 RAMACHANDRAN, G. N. & WOOSTER, W. A. (1950). *Acta Cryst.* **3**, 73.
 SEN, R. K. (1949). *Acta Cryst.* **2**, 127.

Acta Cryst. (1950). **3**, 242

Crystallography of rhombohedral sulfur. By CLIFFORD FRONDEL and R. E. WHITFIELD, *Harvard University, Cambridge, Mass., U.S.A.*

(Received 13 December 1949)

The existence of a rhombohedral polymorph of sulfur has been earlier established by Engel (1891) and by Aten (1914). Friedel (1891) found Engel's crystals to be hexagonal prisms terminated by a flat rhombohedron. Crystals prepared by one of us (R.E.W.) using Aten's method of crystallization from toluene solution were hexagonal prisms doubly terminated by a rhombohedron with $\rho = 24^\circ 25' \pm 15'$. During crystallization, both the rhombohedral and orthorhombic polymorphs may deposit

simultaneously, together with films of plastic sulfur. The rhombohedral crystals have an orange-yellow to pale orange-brown color, and differ in this respect from the greenish yellow to yellow color of the orthorhombic polymorph. No cleavage was observed and the fracture is uneven to subconchoidal. The hardness is about 2. Optically the crystals are uniaxial negative and are weakly dichroic with absorption $O > E$. Study of the crystals is greatly hindered by the rapidity with which they break