

necessity to extend the scope of crystal-structure investigations from the use of prism-zone data only to the use of all of the general reflections makes such a method desirable. The method makes use of but two IBM machines, viz. a hand key punch and a tabulator, the latter preferably equipped with progressive totals.

In the orthogonal crystal systems we have the relation

$$\sin^2 \theta_{hkl} = h^2 \lambda^2 / 4a^2 + k^2 \lambda^2 / 4b^2 + l^2 \lambda^2 / 4c^2.$$

If values of  $1/d^2$  are desired, the factor  $\lambda^2/4$  is omitted from each term. Three small decks of cards are first prepared with the hand punch; these are designated  $(2h-1)\sin^2\theta_{100}$ ,  $(2k-1)\sin^2\theta_{010}$  and  $(2l-1)\sin^2\theta_{001}$ , where  $h$ ,  $k$  and  $l$  run from 1 to their respective maximum observed values. Deck 1 is punched 1 in col. 1,  $(2h-1)$  in cols. 4-5, and  $(2h-1)\sin^2\theta_{100}$  in cols. 10-15; deck 2 is punched 1 in col. 2,  $(2k-1)$  in cols. 6-7, and  $(2k-1)\sin^2\theta_{010}$  in cols. 10-15; deck 3 is punched 1 in col. 3,  $(2l-1)$  in cols. 8-9, and  $(2l-1)\sin^2\theta_{001}$  in cols. 10-15. Columns 1, 2, 3, 4-5, 6-7, 8-9 and 10-15 are then wired to add in separate counters. If we now pass deck 1 through the tabulator, and take progressive totals, we obtain directly the values of  $\sin^2\theta_{h00}$ , since  $\sum_{n=1}^h (2n-1) = h^2$ . The process is now repeated after adding to the deck the first  $(2k-1)\sin^2\theta_{010}$  card. We now obtain values of  $\sin^2\theta_{h10}$ . The  $\sin^2\theta$  values for the planes  $h20$ ,  $h30$ , ...,  $h01$ ,  $h11$ , ...,  $h02$ ,  $h12$ , etc., are then obtained by continuing the process of adding the proper next card after each pass of the deck. In the general case, the totals in the counters will be  $h$ ,  $k$ ,  $l$ ,  $h^2$ ,  $k^2$ ,  $l^2$ ,  $\sin^2\theta_{hkl}$ . The squares of the Miller indices are printed as a check to insure that the cards in each deck were fed in the proper

order, since the printed indices themselves are simply counts of the number of cards in each deck. By keeping watch on the value of  $\sin^2\theta$  for  $(h_{\max}, k_l)$  in each group it is possible to remove cards from the back of the

$$(2h-1)\sin^2\theta_{100}$$

deck in order to keep all the values calculated below a pre-determined maximum, this value being unity if data for all planes within the sphere of reflection are desired.

If the tabulator does not have progressive totals, the same method may be used, but in this case each value of  $\sin^2\theta$  to be computed requires a separate pass of the deck through the machine, and the handling of cards is considerably increased.

This method may be extended for use in the hexagonal and monoclinic systems, in which

$$\sin^2\theta = \frac{\lambda^2 h^2}{4a^2} \sin^2\beta + \frac{\lambda^2 k^2}{4b^2} + \frac{\lambda^2 l^2}{4c^2} \sin^2\beta - \frac{\lambda^2 hl \cos\beta}{2ac \sin^2\beta}.$$

The procedure with the first three terms is identical with that outlined above; the last term requires the punching of an additional deck with values of  $A_i \lambda^2 \cos\beta / 2ac \sin^2\beta$ , the values of  $A_i$  being chosen so that combinations of them will form all observed  $(hkl)$  combinations. By proper wiring, values of  $\sin^2\theta$  for  $(hkl)$  and  $(\bar{h}\bar{k}\bar{l})$  may be obtained simultaneously.

We have used this method in the calculation of complete  $\sin^2\theta_{hkl}$  values for four different crystals. As an illustration of the saving of time effected, a recent calculation of the complete set of over 3000 values inside the Cu  $K\alpha$  sphere of reflection for an orthorhombic cell which has  $a=11$ ,  $b=13$  and  $c=16$  A. took about 4 hr.

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**Errata in Lonsdale's Structure Factor Tables.** By K. LONSDALE. *Chemistry Department, University College, Gower Street, London W.C.1, England*

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In rearranging the structure factor tables for Volume 1 of the new *International Tables*, I have found the following errata, which should be noted by those who are now using the existing *Structure Factor Tables*. I should be most grateful for information of other corrections, if any.

p. 15.  $Pc$ ,  $l=2n$ :

$$" \alpha(\bar{h}kl) = -\alpha(h\bar{k}l) = \alpha(hkl) "$$

should read  $" \alpha(\bar{h}kl) = -\alpha(h\bar{k}l) \neq \alpha(hkl) "$ .

$Pc$ ,  $l=2n+1$ :

$$" \alpha(\bar{h}kl) = -\alpha(h\bar{k}l) "$$

should read  $" \alpha(\bar{h}kl) = \pi - \alpha(h\bar{k}l) "$ .

p. 16.  $Cc$ ,  $l=2n+1$ :

$$" \alpha(\bar{h}kl) = -\alpha(h\bar{k}l) "$$

should read  $" \alpha(\bar{h}kl) = \pi - \alpha(h\bar{k}l) "$ .

p. 20.  $Pmc$ ,  $l=2n+1$ :

$$" \alpha(hkl) = \dots = \pi - \alpha(h\bar{k}l) "$$

should read  $" \alpha(hkl) = \dots = \pi - \alpha(hkl) "$ .

p. 26.  $Abm$ ,  $k=2n+1$ :

Delete "or  $k=0$ ".

$Ama$ ,  $h=2n+1$ :

Delete " $h=0$  or".

p. 27.  $Fdd$ :

Add } at end of formulae for  $A$  and  $B$ .

p. 29.  $Ima$ ,  $h=2n+1$ :

Delete " $h=0$  or".

p. 64.  $I\bar{4}c2$ , bottom of page:

Delete " $A'=0$  if  $h=\pm k$ ".

p. 80.  $I42$ , last set of coordinates:

" $yx\bar{z}$ " should read " $\bar{y}xz$ ".

p. 94.  $R\bar{3}$ ,  $h-k+l=3n$ :

Add ] at end of line.

p. 105. Second line:

Add } at end of line.

p. 115.  $C\bar{6}c2$ ,  $l=2n+1$ :

$$" \alpha(\bar{h}kl) = \pi - \alpha(hkl) "$$

should read  $" \alpha(\bar{h}kl) = \pi - \alpha(h\bar{k}l) "$ .

p. 121.  $C6_12$ ,  $l=6n+1$ :

$$" B = 2\{\cos[\sin - \sin] + \sin[\sin - \sin] + \sin[\sin - \sin]\} "$$

should read

$$" B = 2\{\cos[\sin - \sin] + \cos[\sin - \sin] + \cos[\sin - \sin]\} "$$

- p. 135.  $F43m$ ,  $h+k=2n$  and  $k+l=2n$ :  
Delete "As for  $P43m$ " and substitute "A and B as for  $P43m$  (page 134), but with numerical factor 16 instead of 4".  
 $I43m$ ,  $h+k+l=2n$ :  
Delete "As for  $P43m$  (page 134)" and substitute "A and B as for  $P43m$  (page 134), but with numerical factor 8 instead of 4".
- p. 137.  $F43c$ ,  $h+k=2n$ ,  $k+l=2n$ ,  $l=2n$ :  
Delete "As for  $P43n$  (1) (page 136)" and substitute "A and B as for  $P43n$  (1) (page 136), but with numerical factor 16 instead of 4".  
 $F43c$ ,  $h+k=2n$ ,  $k+l=2n$ ,  $l=2n+1$ :  
Delete "As for  $P43n$  (2) (page 136)" and substitute "A and B as for  $P43n$  (2) (page 136), but with numerical factor 16 instead of 4".  
 $I43d$ ,  $h+k+l=4n$ ,  $h=2n$ ,  $k=2n$ :  
Delete "As for  $P43n$  (1) (page 136)" and substitute "A and B as for  $P43n$  (1) (page 136), but with numerical factor 8 instead of 4".
- p. 138.  $I43d$ ,  $h+k+l=4n+2$ ,  $h=2n$ ,  $k=2n$ :  
Delete "As for  $P43n$  (2) (page 136)" and substitute "A and B as for  $P43n$  (2) (page 136), but with numerical factor 8 instead of 4".
- p. 140.  $F43$ ,  $h+k=2n$  and  $k+l=2n$ :  
Delete "As for  $P43$  (page 139)" and substitute "A and B as for  $P43$  (page 139), but with numerical factor 16 instead of 4".
- p. 142.  $I43$ ,  $h+k+l=2n$ :  
Delete "As for  $P43$  (page 139)" and substitute "A and B as for  $P43$  (page 139), but with numerical factor 8 instead of 4".
- p. 144.  $P4_33$ , (6):  
"A = 0 if  $h=0$ ; B = 0 if  $k=0$ "  
should read "A = 0 if  $k=0$ ; B = 0 if  $h=0$ ".
- p. 158.  $Pn\bar{m}n$ , formula for A:  
"h-l" should read "l-h".  
 $Pban$ , bottom line but one:  
Delete "= 0 if  $h=0$  or  $k=0$ ".
- p. 162.  $P4_2/n$ ,  $h+k=2n$ ,  $k+l=2n+1$ :  
Add "A = 0 if  $h=k=0$ ".
- p. 180. Sixth line:  
At end of formula for A the group of brackets  
) should be )].
- p. 181.  $Fd3c$ ,  $h+k=4n$ ,  $k+l=4n+2$ ,  $l+h=4n$ :  
"A = -32{ $\Sigma \sin \sin \cos + \Sigma \cos \sin \sin$ }"  
should read  
"A = -32{ $\Sigma \sin \cos \sin + \Sigma \cos \sin \sin$ }".

I am grateful to Dr Helen Megaw for directing my attention to the first two of the above errata and thereby shattering my complacency in regard to the remainder of the text.

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**Oriented growth of silver in silver halide crystallites.** By D. W. PASHLEY, *Physics Department, Imperial College, London S.W. 7, England*

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In view of the footnote to a recent paper by Berry (1949), a preliminary account of some work in progress in this Department would appear to be of interest.

Berry reports that during the irradiation of a single crystal of silver bromide with a mercury-vapour lamp, oriented growth of silver occurs such that the (110) planes of the two crystals are parallel, but are rotated through 90° with respect to one another. It is also apparent from his work that there is no change in large silver bromide crystals, or in thin oriented layers of silver iodide, during the exposure of the specimens to the electron beam in the diffraction camera; this is in accord with observations by other workers (see, for example, Wilman (1940)).

During the course of an electron-diffraction investigation of completely oriented layers of silver bromide and silver chloride, formed by condensation from the vapour, it has been found, in contrast to the results of Berry and others, that the electron beam causes the halide to change gradually to silver, until only a very small amount of the halide finally remains. Crystal size has a considerable influence on the halide stability, since it is found that the thinnest layers studied, only a few Ångström units thick, change far more rapidly under the electron beam than do those of several hundred Ångström units thickness.

During the early stages of decomposition of the silver chloride, the silver grows in an orientation completely parallel to that of the chloride (both crystals being cubic), and as the process continues prominent streaks appear on the electron-diffraction patterns, parallel to the [111] directions in the silver crystals. These streaks seem to indicate either a growth in the form of thin (111) plates of silver, or some form of distortion occurring perpendicular to the silver (111) planes. Extra spots later appear on these streaks, indicating that the silver is twinning about all of its [111] axes.

During the decomposition of the bromide layers, parallel growth of silver also occurs, although more polycrystalline silver is formed than in the chloride case, and other weaker orientations of the silver also appear.

When the halide layers are formed by chemically attacking surfaces of silver single crystals, they are stable to the electron beam. Such halide layers have been reduced by means of a photographic developer, when much of the silver produced grows orientated parallel to the large silver crystals and is twinned about its [111] axes; this growth is independent both of the orientation of the surface of the silver crystal and of the relative orientations of the silver and silver halide. Similar growth also occurred