

It is of interest to examine the results of Chandrasekaran (1959) in the light of the present point of view. He measured values of  $\alpha$  in a number of cases in the hope that it would be a suitable measure of the perfection of the crystals studied. If  $\alpha$  traversed a smooth curve between  $\alpha_p$  and  $\alpha_m$ , it would indeed be suitable, but the form of the dashed curve in Fig. 1 shows that  $\alpha$  is not a good measure of perfection. As a matter of fact, Chandrasekaran gives data which support the general form of the dashed curve. In one case for  $S=(0.10)S_m$  he found  $\alpha=(1.06)\alpha_p$ , and in another for  $S=(0.26)S_m$  he found  $\alpha=(0.98)\alpha_p$ . The corresponding enhancement factors were 20 and 6, and these were the two largest enhancement factors which he studied. These cases had different values of  $2\theta_M$ , but this does not affect the general argument greatly, as was pointed out above.

In conclusion, it should be pointed out that the important consideration is the fact that we have measured the value of the polarization ratio of a monochromated beam for an actual apparatus using an accurate technique. The value obtained not only is not close to that appropriate to a mosaic monochromator, but is not even in the range between such a value and that calculated for a perfect monochromator. Using the mosaic value may lead to an error in the polarization factor of up to 15%. This result

has important applications to any study of the angular dependence of monochromatic X-ray scattering, no matter what the form of the sample, for both Bragg and diffuse scattering, and regardless of the position of the monochromator with respect to the sample. In fact, it may be necessary to use these considerations for reflections of unpolarized radiation which suffer appreciable extinction. The validity of the plausibility arguments given to explain the situation do not alter the necessity of accepting the measured value of polarization ratio.

I should like to thank Drs D.R. Chipman and C.B. Walker for discussion and comments on the manuscript.

#### References

- BACON, G. E. & LOWDE, R. D. (1948). *Acta Cryst.* **1**, 303.  
 CHANDRASEKARAN, K. S. (1959). *Acta Cryst.* **12**, 916.  
 CHIPMAN, D. R. & BATTERMAN, B. W. (1963). *J. Appl. Phys.* **34**, 912.  
 MIYAKE, S., TOGAWA, S. & HOSOYA, S. (1964). *Acta Cryst.* **17**, 1083.  
 Powder Intensity Project (1967). *Acta Cryst.* **23**, 1116.  
 ZACHARIASEN, W. H. (1945). *X-ray Diffraction in Crystals*. New York: John Wiley. See especially equation (4.27).

*Acta Cryst.* (1968). A**24**, 474

**Comments on a paper by Sabine.** By CHARLES A. JOHNSON, *Edgar C. Bain Laboratory for Fundamental Research, United States Steel Corporation, Monroeville, Pennsylvania 15146, U.S.A.*

(Received 7 April 1967 and in revised form 29 January 1968)

A recent calculation of the diffraction effects produced by condensed sheets of interstitial atoms is discussed. An error is pointed out; this error vitiates the calculation.

Sabine (1966) has recently published a calculation of the diffraction effects produced by condensed layers of interstitial atoms in face-centered cubic crystals. His calculation predicts peak shifts which, for small values of the fault probability  $\alpha$ , are opposite to the shifts previously computed for extrinsic faults by Johnson (1963) (for  $0 \leq \alpha \leq 1$ ) and by Warren (1963) (for  $\alpha \ll 1$ ). The results given by Johnson and by Warren agree when  $\alpha \ll 1$ . Sabine notes that in the limit of low fault probability ( $\alpha \ll 1$ ) the diffraction effects produced by condensed interstitial layers should be the same as those produced by extrinsic faults. He does not explain the discrepancy.

I believe that this discrepancy is accounted for by the fact that there is an error in Sabine's calculation. This error is to be found in the difference equation scheme by which Sabine computes the probabilities of the possible stacking sequences. (Since we are particularly interested in case  $\alpha \ll 1$ , Sabine's parameter  $\beta = \alpha/(1 + \alpha)$  will be used interchangeably with  $\alpha$ .)

Suppose that a given layer is *A*. If this layer is part of the original crystal then the probability that the next layer will be *B* is  $(1 - \beta)$ . But if this *A* layer is a *condensed* layer then the probability that the next layer will be *B* is  $\beta$ . [For suppose that this *A* layer is the only condensed layer in the

crystal (so that  $\beta \rightarrow 0$ ); in this case the next layer is *necessarily* *C*.] This distinction between original and condensed planes is shown in Sabine's 'probability tree'. Unfortunately, Sabine's difference equation scheme does not incorporate this distinction between original and condensed layers. Specifically, the 'additional relation'

$$P_m^A = \beta P_{m-1}^B + (1 - \beta) P_{m-1}^C \quad *$$

is true only if the  $(m - 1)$  layer is part of the original crystal. If the  $(m - 1)$  layer is a *condensed* layer this relation must be changed to

$$P_m^A = (1 - \beta) P_{m-1}^B + \beta P_{m-1}^C$$

This difficulty seems to be insurmountable in the difference equation approach used, and clearly vitiates Sabine's subsequent results for all values of the fault probability.

The inherent difficulty in applying such a difference equation scheme to this problem can be seen as follows. There are, allowing for normalization of the probabilities to unity, two independent probabilities for the stacking of

\* There is a typographical error in this equation in Sabine's paper. The last term should read  $(1 - \beta) P_{m-2}^C$ . Sabine's subsequent equations follow only if this correction is made.

the  $m$ th layer, say  $P_m^A$  and  $P_m^B$ , which must be computed. This requires two equations relating  $P_m^A$  and  $P_m^B$  to the corresponding quantities for the layers  $(m-1)$  and  $(m-2)$ , respectively. These two equations (which are to hold for all  $m$ ) must be mutually consistent. That is, given values of say,  $P_5^A$  and  $P_5^B$  we can compute  $P_7^A$  and  $P_7^B$  either by a single application of the equation relating the  $(m)$  and  $(m-2)$  layers, or by repeated application of the equation relating the  $(m)$  and  $(m-1)$  layers and we must of course get the same answer either way. The difference equations given by Sabine are not consistent in this sense.

The possibility of this sort of internal inconsistency arises from the fact that the problem has been overspecified. The diffraction effects are determined by the *relative* positions of the layers, and the relative positions are determined by

the stacking sequence written in terms of Frank's (1951) transition symbols  $\Delta$  and  $\nabla$ . Allowing for normalization of probabilities there is then only one variable,  $P_m^\Delta$ , the probability that the  $m$ th transition be  $\Delta$ ; only one difference equation need be written, and the possibility of internal inconsistency thus disappears. However, the construction of a suitable equation for the problem in question appears to be very difficult.

### References

- FRANK, F. C. (1951). *Phil Mag.* **42**, 809.  
 JOHNSON, C. A. (1963). *Acta Cryst.* **16**, 490.  
 SABINE, T. M. (1966). *Acta Cryst.* **21**, 882.  
 WARREN, B. E. (1963). *J. Appl. Phys.* **34**, 1973.

*Acta Cryst.* (1968) **A24**, 475

**Reply to 'Comments on a paper by Sabine'.** By T. M. SABINE\*, *Department of Physics, Brookhaven National Laboratory, Upton, L. I., New York 11973, U.S.A.*

(Received 1 November 1967 and in revised form 2 April 1968)

An objection to the treatment of the problem of the diffraction of X-rays by crystals containing condensed sheets of interstitial atoms is discussed.

Johnson (1968) has concluded that my calculation of the diffraction effects produced by condensed sheets of interstitial atoms in a face-centred cubic crystal is in error.

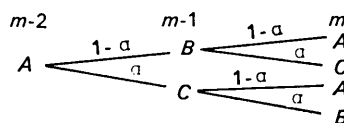
The calculation is certainly not exact in that, as Johnson points out, vectors originating on condensed layers have been ignored. This should not seriously affect the results for  $\alpha$  small in that in the computation of the Patterson function for any value of the interlayer spacing the numbers of vectors from uncondensed to uncondensed layers, from uncondensed layers to condensed layers and condensed to condensed layers are in the ratio  $(1-\alpha)^2:2\alpha(1-\alpha):\alpha^2$ , and the major contribution to the average value of the structure factor product will come from the product for uncondensed to uncondensed layers. Warren (1963) makes a less severe approximation in his treatment of the double deformation fault problem, by neglecting terms due to vectors from layers in a fault to those in another fault.

The second difficulty is more serious and could vitiate the calculation, although Sato (1966) solved the triple fault problem by difference equations and a recent calculation by Kakinoki (1967) confirms his result as well as Johnson's result for the double deformation fault problem.

If Johnson's statement that the relationship between the  $m$ th and  $(m-2)$ th layer should be the same whether obtained directly or by applying the relationship between the  $m$ th and  $(m-1)$ th layers twice then only the deformation fault problem (Paterson, 1952) can be treated by the method of probability trees used by Warren (1959) since the relationship between the  $(m-2)$ th and  $(m-1)$ th layer is identical in all problems. To illustrate this the four classic problems will be considered. In each case  $\alpha$  is the appropriate faulting parameter.

#### (1) Growth faults in h.c.p. crystals (Wilson, 1942)

Wilson's difference equation is generated by the trees



and its cyclic permutations through the relations

$$P_m^A = (1-\alpha)P_{m-2}^A + \alpha(1-\alpha)P_{m-2}^B + \alpha^2 P_{m-2}^C \quad (1.1)$$

$$P_{m-1}^A = (1-\alpha)P_{m-2}^C + \alpha P_{m-2}^B \quad (1.2)$$

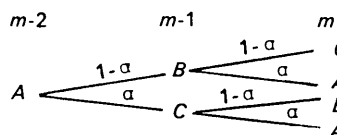
$$P_{m-2}^A + P_{m-2}^B + P_{m-2}^C = 1 \quad (1.3)$$

When the boundary conditions

$P_0^A = 1$ ,  $P_1^A = 0$  and  $P_0^B = 0$ ,  $P_1^B = \frac{1}{2}$  are used Wilson's result is obtained even though the second boundary condition is inconsistent with the tree.

#### (2) Growth faults in f.c.c. crystals (Paterson, 1952)

Paterson's difference equation is generated by the tree (also used by Sabine, 1966)



and its cyclic permutations through the relations

$$P_m^A = \alpha P_{m-2}^A + (1-\alpha)^2 P_{m-2}^B + \alpha(1-\alpha) P_{m-2}^C \quad (2.1)$$

and (1.2) and (1.3). Using identical boundary conditions to (1) Paterson's result is obtained.

\* Present address: A.A.E.C. Research Establishment, Lucas Heights, N.S.W. 2232, Australia.