the mth 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 $\triangle$ and $\triangledown$. Allowing for normalization of probabilities there is then only one variable, $P_m\triangle$, the probability that the mth transition be $\triangle$; 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.

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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.*

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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.

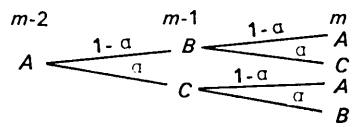
The calculation is certainly not exact in that, as Johnson points out, vectors originating on condensed layers have been ignored. This should not seriously affect the results for α small in that in the computation of the Patterson function for any value of the interlayer spacing the numbers of vectors 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 mth and $(m-2)$th layer should be the same whether obtained directly or by applying the relationship between the mth 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 α 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

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

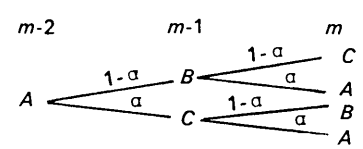
$$P_{m-1}^A=(1-\alpha)P_{m-2}^C+\alpha P_{m-2}^B \qquad (1.2)$$

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

When the boundary conditions $P_0^A=1, P_1^A=0$ and $P_0^A=0, P_1^A=\frac{1}{2}$ 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

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

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

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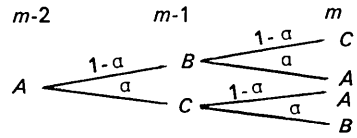
(3) *Single deformation fault in f.c.c. crystals* (*Paterson*, 1952). In this case the tree is

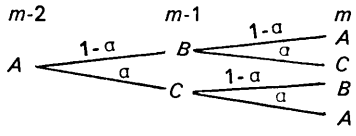


plus its cyclic permutations and Paterson's equation is given by

$$P_m^A = 2\alpha(1-\alpha)P_{m-2}^A + (1-\alpha)^2 P_{m-2}^B + \alpha^2 P_{m-2}^C \quad (3.1)$$

plus (1.2) and (1.3.) Application of boundary conditions $P_0^A = 1$, $P_1^A = 0$ and $P_0^B = 1$, $P_1^A = \alpha$; $P_0^C = 1$ $P_1^A = 1-\alpha$, which are consistent with the tree give Paterson's solution. Equation (3.1) is also obtained by the application of (1.2) twice and (1.3) and is the equation always obtained when (1.2) is applied twice.

(4) *Deformation faults in h.c.p. crystals* (*Christian*, 1956). For this fault the tree is



plus its cyclic permutations and Christian's difference equation is found from

$$P_m^A = (1-2\alpha+2\alpha^2)P_{m-2}^A + \alpha(1-\alpha)(P_{m-2}^B + P_{m-2}^C) \quad (4.1)$$

and (1.3). In this case there is no relation between adjacent layers however. Warren (1958) used (1.2) for the combined deformation and growth fault in h.c.p. crystals.

The boundary conditions

$$P_0^A = 1,\ P_1^A = 0; \quad P_0^A = 0,\ P_1^A = \tfrac{1}{2}$$

lead to Christian's result.

It seems therefore that if Johnson's conclusion that the problem is overspecified is correct only one of these problems can be solved by probability tree methods.

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Elimination of harmonic radiation in thermal diffuse X-ray scattering measurements.*

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A method is presented for determining the effectiveness of proportional counter descrimination against harmonic radiation passed by a crystal monochromator in X-ray studies. A method is also given for correcting for this contamination in thermal diffuse scattering experiments where such effects may be important.

When a crystal monochromator is employed in X-ray measurements a proportional counter and pulse height analyzer (PHA) may be used to discriminate against the harmonic radiation passed by the monochromator. An oriented single crystal in the sample position can be used to determine the effectiveness of this discrimination with the method to be described. This method, applied to three commercially available proportional counter systems, has shown that such systems have varied capabilities in this regard, and that effective discrimination cannot be reliably predicted on the basis of electronic pulse amplitude discrimination alone. Finally, a method is described for correcting the count rate in those situations where the discrimination against the harmonic radiation proves inadequate.

We consider only the $\lambda/2$ harmonic, where λ is the design wavelength of the monochromator. If the $\lambda/2$ diffraction vector is set on a point in the reciprocal lattice of the sample crystal in such a way that the λ diffraction vector is not on a reciprocal lattice point then the $\lambda/2$ radiation will be Bragg reflected and the scattering of the λ radiation will be relatively much weaker. Take as the quantity of interest the fraction f of the incident $\lambda/2$ radiation which results in pulse heights lying within the PHA window used for λ pulses. The wavelength dependence of absorption is used to determine f as follows. Let α_1 and α_2 be the fractions of the λ and $\lambda/2$ radiation, respectively, which is transmitted by an absorbing foil. The count rate $(\alpha I)_{\exp}$ is measured with foil in place, using the PHA window customarily employed for the λ radiation. Similarly $I_{\exp}$ is measured at the same point without the foil. Then

$$(\alpha I)_{\exp} = \alpha_1 I_1 + \alpha_2 f I_2$$
$$I_{\exp} = I_1 + f I_2$$

where I_1 and fI_2 are the λ and $\lambda/2$ contributions respectively. Eliminating I_1 gives

$$fI_2 = \frac{(\alpha I)_{\exp} - \alpha_1 I_{\exp}}{\alpha_2 - \alpha_1}.$$

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