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X-ray Diffraction by Stacking Faults in H.C.P. or F.C.C. Crystals

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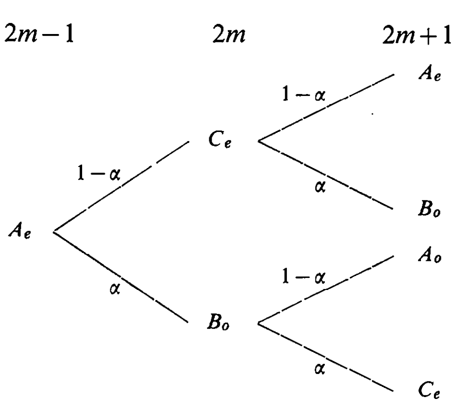
Probability trees and difference equations relating adjacent layers are given for C and CC faults in h.c.p. crystals and H faults in f.c.c. crystals.

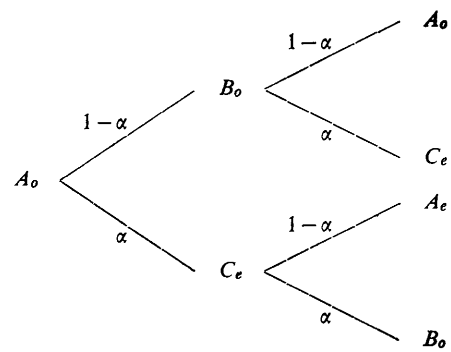
Introduction

Sabine (1968) has recently given difference equations for the four classic cases of C (growth) and CC (deformation) faults in h.c.p. crystals and H (growth) and HH (single deformation) faults in f.c.c. crystals. (See Nabarro, 1967, for fault notation.) The difference equations are, however, not self-consistent in the sense that a single application of the equation relating layers m and $(m-2)$ does not give the same result as successive application of the equation relating layers m and $(m-1)$ (Johnson, 1968), except for the case of HH faults in f.c.c. crystals. We shall show below that it is possible to obtain self-consistent difference equations for the other three cases. In what follows, we assume that, in the absence of a fault, the transition from the layer 0 to 1 is of the type Δ (Frank, 1951). In each case α is the appropriate faulting parameter and the P's are the probabilities of obtaining the layer type indicated in the superscript at the layer indicated in the subscript.

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

It can be easily shown that the probability for the transition Δ or ∇ after the layer m depends on whether m is odd or even, as well as on the odd or even nature of the total number of faults preceding the layer m. Sabine (1968) overlooks both these points in forming the probability tree and in writing equations (1·1) and (1·2). The appropriate probability trees in this case are





and their cyclic permutations. The subscripts e and o refer to the even or odd nature of the total number of faults up to the layer under consideration. The following difference equations are generated by the trees:

$$P^{A_e}_{2m}=(1-\alpha)P^{B_e}_{2m-1}+\alpha P^{B_o}_{2m-1}=(1-2\alpha)P^{B_e}_{2m-1}+\alpha P^{B}_{2m-1}\,, \tag{1}$$

$$P^{A_o}_{2m}=(1-\alpha)P^{C_o}_{2m-1}+\alpha P^{C_e}_{2m-1}=(1-2\alpha)P^{C_o}_{2m-1}+\alpha P^{C}_{2m-1}\,, \tag{2}$$

$$P^{A_e}_{2m-1}=(1-\alpha)P^{C_e}_{2m-2}+\alpha P^{C_o}_{2m-2}=(1-2\alpha)P^{C_e}_{2m-2}+\alpha P^{C}_{2m-2}\,, \tag{3}$$

$$P^{A_o}_{2m-1}=(1-\alpha)P^{B_o}_{2m-2}+\alpha P^{B_e}_{2m-2}=(1-2\alpha)P^{B_o}_{2m-2}+\alpha P^{B}_{2m-2}\,, \tag{4}$$

where P^A_m and its cyclic permutations are defined through equations of the type

$$P^A_m=P^{A_e}_m+P^{A_o}_m\,. \tag{5}$$

Adding equations (1) and (2) and substituting from equation (5) and cyclic permutations of equations (3) and (4), we get

$$P^A_{2m}=(1-2\alpha)P^A_{2m-2}+\alpha(P^B_{2m-1}+P^C_{2m-1})\,. \tag{6}$$

Similarly

$$P^A_{2m-1}=(1-2\alpha)P^A_{2m-3}+\alpha(P^B_{2m-2}+P^C_{2m-2})\,. \tag{7}$$

In general, therefore, we obtain Wilson's difference equation,

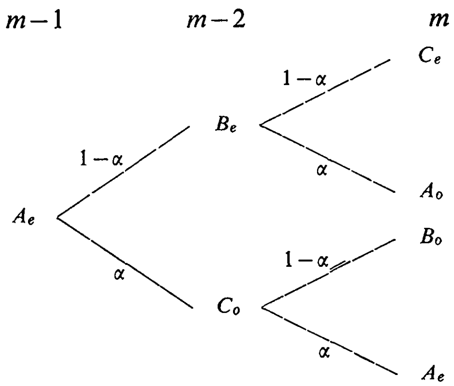
$$P_m^A=(1-2\alpha)P_{m-2}^A+\alpha(1-P_{m-1}^A)\,, \tag{8}$$

since

$$P_{m-1}^A+P_{m-1}^B+P_{m-1}^C=1\,. \tag{9}$$

2. *H* faults in f.c.c. crystals (Paterson, 1952)

The probability of the transition Δ or ∇ after the layer m depends on whether the number of faults preceding the layer m is even or odd. This fact is not considered by Sabine in forming his probability tree. Paterson's difference equation is generated by the tree



and its cyclic permutations through the relations:

$$P_m^{A_e}=(1-\alpha)P_{m-1}^{C_e}+\alpha P_{m-1}^{C_o}$$
$$=(1-\alpha)P_{m-1}^{C}-(1-2\alpha)P_{m-1}^{C_o}\,, \tag{10}$$

$$P_m^{A_o}=(1-\alpha)P_{m-1}^{B_o}+\alpha P_{m-1}^{B_e}$$
$$=(1-\alpha)P_{m-1}^{B}-(1-2\alpha)P_{m-1}^{B_e}\,. \tag{11}$$

Adding equations (10) and (11) and substituting from equations (5) and cyclic permutations of equations (10) and (11) for $P_{m-1}^{C_o}$ and $P_{m-1}^{B_e}$, we get

$$P_m^A=(1-\alpha)\,(P_{m-1}^B+P_{m-1}^C)-(1-2\alpha)P_{m-2}^A\,. \tag{12}$$

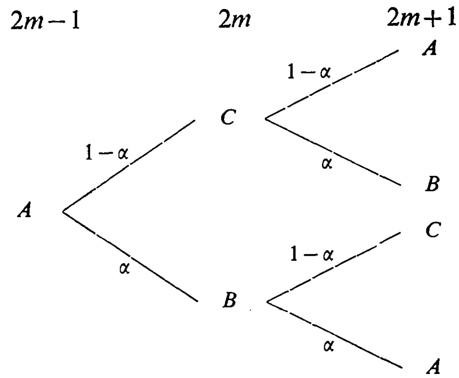
With the use of equation (9), we obtain

$$P_m^A=(1-\alpha)\,(1-P_{m-1}^A)-(1-2\alpha)P_{m-2}^A\,, \tag{13}$$

which is Paterson's difference equation for this case.

3. *CC* faults in h.c.p. crystals (Christian, 1954)

A little consideration shows that the probability of the transition Δ or ∇ after the layer m depends on the odd or even nature of m. The appropriate probability tree



and its cyclic permutations give

$$P_{2m+1}^A=(1-\alpha)P_{2m}^C+\alpha P_{2m}^B\,, \tag{14}$$

$$P_{2m}^A=(1-\alpha)P_{2m-1}^B+\alpha P_{2m-1}^C\,. \tag{15}$$

Sabine incorrectly states that there is no relation between adjacent layers in this case. Substituting from cyclic permutations of equation (15) in equation (14), we have

$$P_{2m+1}^A=(1-2\alpha+2\alpha^2)P_{2m-1}^A+\alpha(1-\alpha)\,(P_{2m-1}^B+P_{2m-1}^C)\,. \tag{16}$$

Similarly

$$P_{2m}^A=(1-2\alpha+2\alpha^2)P_{2m-2}^A+\alpha(1-\alpha)\,(P_{2m-2}^B+P_{2m-2}^C)\,. \tag{17}$$

With the use of equation (9), we obtain in general

$$P_m^A=(1-3\alpha+3\alpha^2)P_{m-2}^A\,. \tag{18}$$

This is Christian's difference equation.

Conclusion

We have shown that it is possible to write difference equations relating adjacent layers and further that these are sufficient for the solution of the four classical problems of faults in h.c.p. and f.c.c. structures. In the way illustrated for *CC* faults in h.c.p. structures, it can be shown in general that the difference equations relating adjacent layers given by us are consistent with those relating alternate layers. Clearly, use of both the difference equations leads to an over-specification of the problem.

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