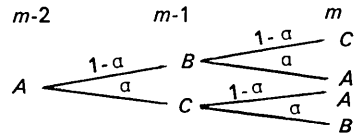
(3) *Single deformation fault in f.c.c. crystals* (*Paterson*, 1952). In this case the tree is

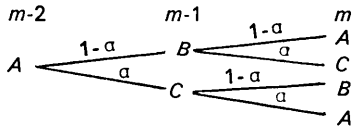


plus its cyclic permutations and Paterson's equation is given by

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

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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(*Received* 5 *May* 1967, *and in revised form* 11 *January* 1968)

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

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

* Work supported in part by the Atomic Energy Commission and the Research Corporation.

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The entire procedure is repeated with an integral mode PHA setting with the baseline above the λ window so as to accept only the $\lambda/2$ radiation and this yields I_2 without f. In this manner f is determined. (Extension of the method to higher harmonics, if important, may be possible by using several foils of varying thickness.)

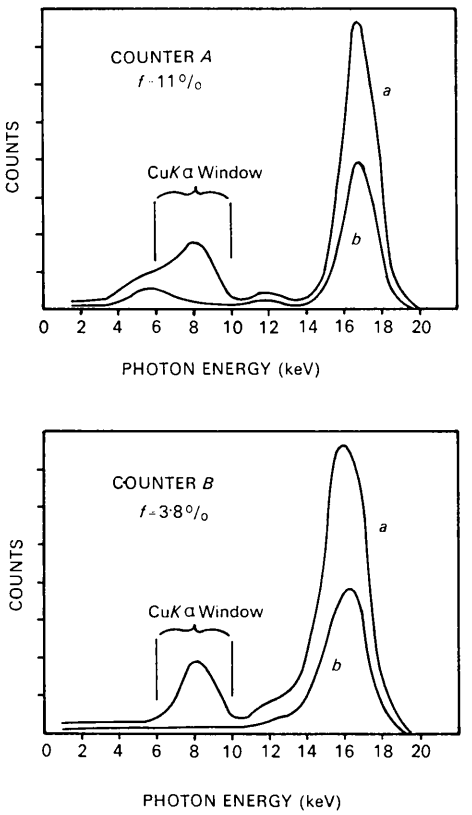

Fig. 1.

Having once determined f one may then correct thermal diffuse scattering (TDS) data obtained in a region where the $\lambda/2$ contribution is important by scanning the region using the integral mode to determine the angular dependence of I_2. Then fI_2 is subtracted from the observed TDS count rate at each angle. One advantage of the method is that the I_2 count rates are relatively high using the integral mode so that the machine time involved in obtaining correction data is short compared with the time spent accumulating TDS data.

The fractions f determined for three different commercial detectors, (xenon filled proportional counters and pre-amps.) were 3·8%, 5·5% and 11%. Their 'resolutions', as judged by the width of the $\lambda/2$ line, were all comparable. Fig. 1 shows how these differences may arise. The curves are PHA scans for two of the counters, the signal being obtained from a Cr(200) reflection for the $\lambda/2$ wavelength TDS only for λ) with a Cu anode tube using a doubly bent lithium fluoride monochromator designed for Cu $K\alpha$ radiation. The scans labeled (*a*) are without absorbing material and those labeled (*b*) were taken with an absorber which passes about 48% of the $\lambda/2$ and 3% of the λ radiation. The peaks at 8 keV in the (*a*) scans are due to the TDS of the characteristic radiation. The peak at 5 keV for counter *A* is only attenuated by a factor of 2 by the absorber so that this portion of the pulse height distribution must be associated with the incident $\lambda/2$ radiation. We attribute this peak to Fe fluorescence from the back wall of the proportional counter, which in this model does not have a double window. It is this peak which accounts for the poor performance of counter *A*.

Finally, it should be noted that the number f depends on the choice of PHA settings used in its determination so that consistent settings must be used. For the f numbers quoted the λCu $K\alpha$ window was between 6 and 10 keV and the integral mode data was taken with a baseline at 10 keV.

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The atomic mechanism of the body-centred cubic to σ-phase transformation. Corrections.

By W. J. KITCHINGMAN, *Metallurgy Department, Institute of Science and Technology, Sackville Street, Manchester* 1, *England*

(*Received* 30 *March* 1968)

orrections to *Acta Cryst.* (1968), A**24**, 282.

The following corrections should be made in the article (Kitchingman, 1968) published under the above title:

Fig. 7, page 286: In the section labelled ATOM in the table, position *C* should be shown as occupied by Nb and position *D* by Al, in the second column.

Page 285, column 2, lines 20–25 should read:

Similarly in the case of 2NbAl incompatibility occurs in the replacement $C \rightarrow D$ and $B \rightarrow D$, since aluminum atoms of coordination number 12 must be replaced by niobium atoms of coordination numbers 14 and 15. Aluminum shows only coordination number 12 and niobium coordination numbers 14 and 15 in the structure.

Reference

KITCHINGMAN, W. J. (1968). *Acta Cryst.* A**24**, 282.