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Concerning an unnecessary approximation made by Zachariasen in treating the perfect-crystal Bragg case.

By S. W. WILKINS, *Division of Chemical Physics, CSIRO, PO Box 160, Clayton, Victoria, Australia 3168*

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An approximation in Zachariasen's [*Theory of X-Ray Diffraction in Crystals* (1945). New York: John Wiley] treatment of X-ray diffraction from a perfect plane-parallel crystal in the Bragg case is pointed out and eliminated. The corresponding unapproximated expression for the transmitted beam is also given. It transpires that Zachariasen's approximation leads to significant errors for 'thin' crystals (*i.e.* those for which the path length is less than or of the order of the extinction length). Some illustrations of the nature of the error are given.

In the course of some calculations it has come to our notice that there is an unnecessary approximation in Zachariasen's (1945) equation (3.139), which, from the text, might be thought to give the general solution for the diffraction of X-rays from a perfect plane-parallel crystal in the Bragg case, treated within the framework of Zachariasen's explicit assumptions. The nature of the approximation is such that it only leads to significant errors for 'thin' crystals (*i.e.* those for which the path length is less than or of the order of the extinction length) and then, apparently only when ψ''_H (or F''_H) is non-zero (for a review concerning another unnecessary approximation introduced by Zachariasen, see Fingerland, 1971).

As Zachariasen's book is widely used as a source for results of X-ray dynamical theory and also because, to our knowledge, the general solution for the Bragg case has not been given in the same convenient form elsewhere, it seems worthwhile to present the unapproximated expression for the diffracted-beam intensity. In addition, we also give the corresponding unapproximated result for the transmitted beam, which is not given by Zachariasen.

Following Zachariasen's notation, we find on substituting for x_1, x_2, c_1 and c_2 in his equation (3.137) that the diffracted intensity is given without approximation by

$$\frac{I_H}{I^e_o} = \frac{b^2|\psi_H|^2[\sin^2 av + \sinh^2 aw]}{D}, \quad (1)$$

where the denominator

$$\begin{aligned} D = {} & |q+z^2| + \{|q+z^2| + |z|^2\}\sinh^2 aw \\ & - \{|q+z^2| - |z|^2\}\sin^2 av + \mathrm{Re}(-z^*u)\sinh(2aw) \\ & + \mathrm{Im}(z^*u)\sin(2av), \end{aligned} \quad (2)$$

while

$$u \equiv v + iw \equiv (q+z^2)^{1/2} \quad (3)$$

and an asterisk denotes the complex conjugate.

Expression (1) may be shown to agree with that given by Zachariasen but for the question of the signs in the fourth and fifth terms in the denominator D. More specifically, Zachariasen effectively takes the moduli of these terms. Following some careful analysis, we find that, at least for the centrosymmetric case, Zachariasen's choice of sign for the fourth term is correct, but that his corresponding treatment of the fifth term in (2) is not valid if

$$\kappa \equiv \frac{\psi''_H}{\psi'_H} \equiv \frac{F''_H}{F'_H} \neq 0, \quad (4)$$

when the fifth term may become negative. The fifth term in (2) only makes a significant contribution for path lengths which are less than or of the order of the extinction length (*i.e.* $A \lesssim \pi$).

The transmitted beam intensity is similarly found from Zachariasen's equation (3.138) to be

$$\frac{I^o_e}{I^e_o} = \frac{|q+z^2|\exp\{-2a\beta\,\mathrm{Im}(z)\}}{D}, \quad (5)$$

where the asymmetry parameter β is given by

$$\beta = \frac{b+1}{b-1} \quad \text{with } -1 \le \beta \le 1. \quad (7)$$

and D is again given by (2).

In order to illustrate the nature of the error introduced by Zachariasen's approximation, we have taken the centrosymmetric case and plotted out diffracted- and transmitted-beam rocking curves for various values of the parameters A, g, β and κ. Two illustrative examples are presented in Figs. 1 and 2.

In calculating the reflectivity $R = P_H/P_O$, we have used the standard approximation that $P_H/P_O = I_H/|b|I_O$, which is valid for beam widths which are large compared to the depth of penetration in the crystal. For the transmissivity T we have correspondingly taken $T = I^o_e/I^e_o$. The 'Zachariasen estimate' for T was obtained by substituting Zachariasen's approximation for D in (5).

The diffracted- and transmitted-beam rocking curves presented in Figs. 1 and 2 show that the present expressions based on (2) lead to much smoother behaviour than those based on Zachariasen's approximation for D. Furthermore, the expected complementary behaviour of T and R is exhibited by the present results but is not exhibited by those based on Zachariasen's approximation.

It may be noted that Zachariasen's approximation is valid for all the cases illustrated in his book, but it is not necessarily valid for *all* cases, whereas (2) will always be correct within the framework of Zachariasen's explicit assumptions. Moreover, there does not appear to be any good reason for making Zachariasen's approximation, since D given by (2)

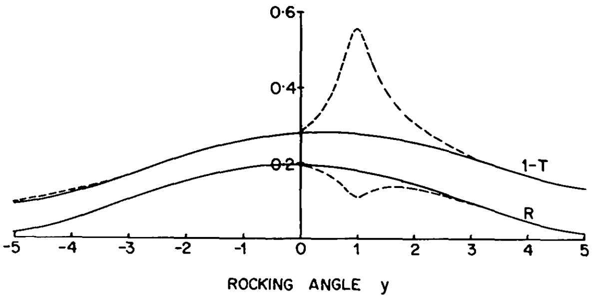

Fig. 1. Reflectivity (R) and transmissivity (T) rocking curves for a centrosymmetric crystal in the *symmetric* Bragg case ($\beta = 0$) plotted against the rocking angle y [defined in equation (3.181) of Zachariasen] for $A = 0{\cdot}5$, $g = -0{\cdot}1$ and $\kappa = +0{\cdot}1$. The solid curves are the solutions given by equations (1) and (2), while the broken curves were obtained by taking Zachariasen's approximation for D.

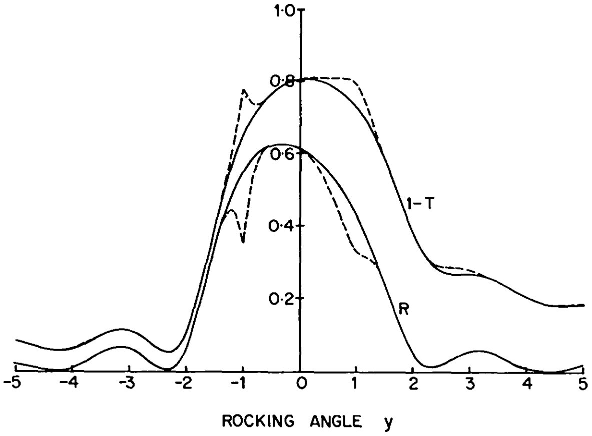

Fig. 2. As for Fig. 1 but with equations evaluated for *asymmetric* Bragg case ($\beta = +0{\cdot}8$) and $A = 1{\cdot}5$, $g(0) = -0{\cdot}1$ [$g(\beta) = g(0)/(1-\beta^2)^{1/2}$] and $\kappa = +0{\cdot}1$.

is just as easy to evaluate as D in Zachariasen's approximation.

In conclusion, we note that the precise form of thin-crystal rocking curves is currently of practical interest. For example, Kohra (1972) and his group have measured (virtually intrinsic) thin-crystal rocking curves for Si.

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On extrinsic faults in face-centred cubic crystals.

By HIDEWO TAKAHASHI, *Faculty of Education, Kagoshima University, Kagoshima, Japan*

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Application of the matrix intensity equation of X-ray diffraction is discussed for the second problem of extrinsic faults in face-centred cubic crystals, discussed by Howard [*Acta Cryst.* (1977), A**33**, 29–32]. The second problem is generalized to the case that the probability with which inserted layers follow layers of the original crystal differs from that with which inserted layers follow previously inserted layers. The **Q** matrix for the case is obtained and the results of intensity calculation are shown.

Recently, Howard (1977) solved the second problem of extrinsic faults in face-centred cubic crystals by the use of the difference equation. We can obtain the same results by application of the matrix intensity equation of X-ray diffraction. Application of the matrix intensity equation to growth, growth and deformation, and multiple-deformation faults in various close-packed structures was discussed by the present author (Takahashi, 1976). Extrinsic faults in f.c.c. crystals are equivalent to double-deformation faults. Our **Q** matrix is different from that of Kakinoki & Komura (1965). As is well known, the **P** matrix is a transition probability matrix of the Markov process. The original definition of the **P** matrix by Kakinoki & Komura (1965) is that the ij element of the **P** matrix is the probability of finding the layer j after the layer i. That is to say, states are defined by kinds of layers in their treatment. States and transition probabilities are called complexions and continuing probabilities, respectively, in this article. Complexions can be defined by sequences of layers or displacement vectors in the matrix intensity equation. If the ith complexion is followed