Short Communications

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Acta Cryst. (1973). A**29**, 215

Reduction of the X-ray intensity equation in matrix form for one-dimensionally disordered structures.

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(*Received* 7 *July* 1971; *accepted* 2 *October* 1972)

The matrices in the X-ray intensity equation for one-dimensionally disordered structures are reduced by taking account of the symmetry character of the matrices.

The intensity equation in matrix form for one-dimensionally disordered structures was given by Hendricks & Teller (1942,) and developed by Kakinoki & Komura (1952, 1954). The equation is expressed as

$$I(\varphi)=N\,\mathrm{spur}\ VF+\sum_{m=1}^{N-1}(N-m)\ \mathrm{spur}\ VFQ^m+\mathrm{conj.}\qquad(1)$$

Allegra (1964) derived an intensity equation which is formally the same as equation (1) but with reduced matrices for the case in which the layers of different kinds are obtained by translations parallel to the layers. In the case of close-packed structures, Kakinoki & Komura (1965) showed that equation (1) can be reduced and that this equation is equivalent to Allegra's if the matrices V, F and Q are put as

$$V=V_0V_0^*\begin{pmatrix} m & \varepsilon^*m & \varepsilon m\\ \varepsilon m & m & \varepsilon^*m\\ \varepsilon^*m & \varepsilon m & m\end{pmatrix}\quad (m)_{ij}=1$$

$$F=\tfrac{1}{3}\begin{pmatrix} w & 0 & 0\\ 0 & w & 0\\ 0 & 0 & w\end{pmatrix}\qquad(2)$$

$$Q=\exp(-i\varphi)P,\ P=\begin{pmatrix} 0 & p_1 & p_2\\ p_2 & 0 & p_1\\ p_1 & p_2 & 0\end{pmatrix}$$

where the elements of matrices V, F and P are minor matrices and $\varepsilon=\exp\{2\pi i(h-k)/3\}$. Then, the spur VFP^m becomes

$$\mathrm{spur}\ VFP^m=V_0V_0^*\ \mathrm{spur}\ mw(\varepsilon p_1+\varepsilon^*p_2)^m\,.\qquad(3)$$

The right-hand side of the equation (3) is found to be equal to Allegra's spur VFQ^m by putting $V_0V_0^*m=V$, $w=F$ and $(\varepsilon p_1+\varepsilon^*p_2)\exp(-i\varphi)=Q$.

By the method of Kakinoki & Komura, however, we can only know that the values of spur VFQ^m in the two equations are identical but cannot know whether the matrices in the two equations are individually equivalent. In general, the equivalence of two matrices means the identity of their eigenvalues. The order of the matrices of equation (1) is three times as large as that of those given by Allegra. Therefore, it is desirable to know not only the identity of spur VFQ^m in both equations but also the identity of the reduced forms of the matrices in equation (1). Since spur VFP^m is a Fourier coefficient of the calculated intensity, the identity of Fourier coefficients of the intensities calculated by both the equations means only the identity of the intensities.

The reduction of the matrix with symmetry may be discussed on the basis of the representation theory of groups. According to this theory, the matrices of the form of (2) have symmetry group C_3 and are reduced by the use of the following T matrix

$$T=\frac{1}{\sqrt{3}}\begin{pmatrix} E & E & E\\ E & \varepsilon_0^*E & \varepsilon_0E\\ E & \varepsilon_0E & \varepsilon_0^*E\end{pmatrix},\qquad(4)$$

where E is the unit matrix of the same order as those of the minor matrices in V, F and P, and $\varepsilon_0=\exp(2\pi i/3)$. As a result we obtain

$$T^{-1}VT=V_0V_0^*\begin{pmatrix} 3m\delta_{h-k,3n} & 0 & 0\\ 0 & 3m\delta_{h-k,3n-1} & 0\\ 0 & 0 & 3m\delta_{h-k,3n+1}\end{pmatrix}$$

$$T^{-1}FT=\frac{1}{3}\begin{pmatrix} w & 0 & 0\\ 0 & w & 0\\ 0 & 0 & w\end{pmatrix}\qquad(5)$$

$$T^{-1}PT=\begin{pmatrix} p_1+p_2 & 0 & 0\\ 0 & {}^*p_1+p_2 & 0\\ 0 & 0 & p_1+{}^*p_2\end{pmatrix}$$

where $\delta_{h-k,3n}$ *etc.* are Kronecker δ's. Hence, a matrix VFP^m can be reduced as

$$VFP^m=V_0V_0^*\ mw(\varepsilon p_1+\varepsilon^*p_2)^m\,,\qquad(6)$$

where ε is 1, ε_0 and ε_0^* according as $h-k$ is $3n, 3n+1$ or $3n-1$. Thus, we can show, by reducing individually the marices V and Q, that Allegra's equation is equivalent to equation (1) in the case of close-packed structure.

The T matrix for the general case discussed by Allegra can be obtained by symmetry considerations of the Q matrix. In Allegra's case, if $V_a^*V_b=V_c^*V_d$, then $p_{ab}=p_{cd}$. Hence, the symmetry of the Q matrix agrees with that of the V matrix. Accordingly, Q and V matrices can be reduced together by the same transformation. If the symmetry group of Q and V matrices is a cyclic group, V can be reduced to a similar form to that in the above case.

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