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## A simplified formula for the calculation of the X-ray intensity diffracted by a monodimensionally disordered structure.

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We have been recently concerned with the calculation of the X-ray intensity diffracted by different models of structures showing disorder with $s=1$ in the stacking of layers. An example is severely ground $\alpha$ (Natta *et al*, 1958) or $\gamma$ (Natta *et al.*, 1959) $TiCl_3$. In the course of our study, we have found a simplified formula for the calculation of the mean intensity diffracted by a single layer.

Mean diffracted intensity is given by:

$$I_{AV}=\sum_1^r if^{(i)}V^{(i)2}+\sum_1^\infty{}_K\sum_1^r{}_{i,j}\mathbf{V}^{(j)*}\mathbf{V}^{(i)}f^{(i)}Q_K^{(ij)} + \sum_1^\infty{}_K\sum_1^r{}_{i,j}\mathbf{V}^{(j)}\mathbf{V}^{(i)*}f^{(i)}Q_K^{(ij)*}; \quad (1)$$

where:

$r$ is the different layers;
$f^{(i)}$ is the frequency of occurrence of the layer of $i$th kind;
$\mathbf{V}^{(i)}$ is the structure factor of the layer of $i$th kind;
$\mathbf{Q}_K$ is the matrix whose $(i,j)$ element is given by the product $P_K^{(ij)}\exp[-i\varphi_K^{(ij)}]$, $P_K^{(ij)}$ being the probability for a layer of the kind $i$ to be followed by a $K$th neighbour of the kind $j$, and $\exp[-\varphi_K^{(ij)}]$ the corresponding fringe factor.

According to Hendricks & Teller (1942), (1) reduces to:

$$I_{AV}=\sum_1^r if^{(i)}V^{(i)2}+\sum_1^r\frac{R^{(ii)}Q^{(i)}}{1-Q^{(i)}}+\sum_1^r i\frac{R^{(ii)*}Q^{(i)*}}{1-Q^{(i)*}}; \quad (2)$$

where $Q^{(i)}$ are the eigenvalues of $\mathbf{Q}_1$, reduced to diagonal form by the similarity operation $\mathbf{OQ}_1\mathbf{O}^{-1}$, and $R^{(ii)}$ are the diagonal elements of the matrix $\mathbf{OVFO}^{-1}$, with $V^{(ij)}=\mathbf{V}^{(i)}\mathbf{V}^{(j)*}$ and $F^{(ij)}=\delta^{(ij)}f^{(i)}$.

It may be possible that the matrix $\mathbf{Q}_1$ cannot be diagonalized, if its eigenvalues are not all different and if $\mathbf{Q}_1$ is not symmetrical.

A new formula for $I_{AV}$, subjected to no conditions of the above type, and simpler than (2), may be derived from (1) in the following way.

Let $\mathbf{V}$ be the row vector:

$$|\mathbf{V}^{(1)}\ldots\mathbf{V}^{(i)}\ldots\mathbf{V}^{(r)}|$$

and $\tilde{\mathbf{V}}$ the corresponding column vector. Remembering that $\mathbf{Q}_K=\mathbf{Q}_1^K$, (1) reduces to:

$$I_{AV}=\sum_1^r if^{(i)}V^{(i)2}+\sum_1^\infty{}_K\mathbf{VFQ}_K\tilde{\mathbf{V}}^*+\sum_1^\infty{}_K\mathbf{V}^*\mathbf{FQ}_K^*\tilde{\mathbf{V}} = \mathbf{VF}\left\{\sum_0^\infty{}_K\mathbf{Q}_1^K\right\}\tilde{\mathbf{V}}^*+\mathbf{V}^*\mathbf{F}\left\{\sum_0^\infty{}_K\mathbf{Q}_1^{K*}\right\}\tilde{\mathbf{V}}-\sum_1^r if^{(i)}V^{(i)2}. \quad (3)$$

But $(\mathbf{Q}_1^K)^{(ij)}$, in the limit of $K\to\infty$, is generally vanishing in whatever statistical structure. Then (3) reduces to:

$$I_{AV}=\mathbf{VF}(\mathbf{E}-\mathbf{Q}_1)^{-1}\tilde{\mathbf{V}}^*+\mathbf{V}^*\mathbf{F}(\mathbf{E}-\mathbf{Q}_1^*)^{-1}\tilde{\mathbf{V}}-\sum_1^r if^{(i)}V^{(i)2}. \quad (4)$$

The only lengthy step in the calculation of $I_{AV}$ through (4) is the evaluation of $(\mathbf{E}-\mathbf{Q}_1)^{-1}$; whereas the calculation of $I_{AV}$ through (2) requires the diagonalization of $\mathbf{Q}_1$, which is not always possible, and the lengthy evaluation of $\mathbf{O}$, $\mathbf{O}^{-1}$, $\mathbf{OVFO}^{-1}$.

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## Neutron diffraction by helical spin structures.

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Recently a new class of magnetic structures, the helical spin structures, has been discussed theoretically (Yoshimori, 1959; Villain, 1959), and a number of experimental examples, for instance in $MnAu_2$ (Herpin *et al.*, 1959) and in metallic holmium (Koehler *et al.*, 1960) has been discovered in neutron diffraction experiments. A simple helical structure may be described as follows: let the ideal lattice sites of the chemical unit cell be described by $\mathbf{r}_k+A_L$ and let us suppose that at each such lattice site is found a magnetic moment $\mu\hat{K}_k^L$ such that all moments make the same constant projection on some crystal direction defined by the unit vector $\hat{u}_3$; that is to say, the moment directions are assumed to be given by

$$\hat{K}_k^L=\cos\beta\hat{u}_3+\sin\beta\hat{u}_k^L, \quad (1)$$

where $\hat{u}_k^L$ is a unit vector normal to $\hat{u}_3$ and $\beta$ is the constant angle between the moment directions and $\hat{u}_3$. It is further assumed that the directions $\hat{u}_k^L$ are described by

$$\hat{u}_k^L=[(\hat{u}_1-i\hat{u}_2)/2\exp i2\pi\boldsymbol{\tau}.(\mathbf{r}_k+\mathbf{A}_L)+\text{C.C.}] \quad (2)$$