The maximum allowable thickness increases either when the accelerating voltage increases or when the unit cell becomes larger. However, the details in the evolution of image contrast with crystal thickness are not the same for these two factors as can be seen by comparing Fig. 4(*a*) with Fig. 4(*c*). This difference is due to the dynamical interaction of Bloch waves in the crystal.

In this paper, we have discussed an accelerating voltage of 1000 kV. In fact, higher voltages such as 3000 kV can be interesting also. A recent discussion on this problem has been given by Jouffrey, Dorignac & Tanaka (1978–1979). However, as most high-voltage microscopes operate at 1000 kV, we have here chosen this voltage for our calculations.

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Simplified Structure Factor for MX_2-Type Compounds

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Abstract

In MX_2-type structures atoms are always in a sandwich form with an M atom surrounded by two X atoms. The orientation of the M atom is always determined by the two X atoms, *e.g.* an M atom with γ orientation will always have two X atoms in A and B (or B and A) orientations around it. Therefore, by representing both X atoms by one M atom, the calculation can be reduced to one third of the original since the summation in the structure-factor calculation over all atoms will reduce to the summation over M atoms only. How this can be done is examined in the paper.

Introduction

The study of polytypism in crystals basically consists of the problem of growth mechanics and the study of

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stacking faults and dislocations. These basic properties can be understood more clearly if the sequence of atoms is known in the crystals. But the determination of the stacking sequence has inherent difficulties in general and in MX_2-types in particular due to the presence of Zhdanov number 1 in the latter types. In any structural determination of an MX_2 (or MX) polytype there are two important steps: spelling out the probable structures; and the calculation of intensities for these probable structures. For the long-period polytypes, both steps are quite lengthy. The number of probable cases depends upon the various clues available in the intensity sequence, while the length of calculations of intensities depends upon the number of atoms in the unit cell. Owing to these difficulties the detailed structure of only 79 polytypes out of 250 in CdI_2 and 17 out of 49 in PbI_2 has been worked out (Trigunayat & Verma, 1976; Jain & Trigunayat, 1978; Jain, Wahab & Trigunayat, 1978; Minagawa, 1979). The calculations in the structure determination of MX_2-type polytypes can be reduced by examining the structure carefully. In MX_2-type structures the atoms are always in a sandwich form, with an M atom surrounded by two X atoms. The orientation of the M atoms is always determined by two X atoms, *e.g.* an M atom at an α orientation will always have two X atoms in B and C (or C and B) orientation around it. In the structure-factor calculation, if we could represent all three atoms by one M atom the calculation would reduce to one third.

Simplified structure factor

The structure factor for any hkl reflection may be written as

$$F_{hkl} = \sum_{p=1}^{n} f_p \exp 2\pi i(hx_p + ky_p + lz_p),$$

the summation being taken over all atoms in the unit cell lying on the vertical A, B, C axes passing through (0,0,0) ($\frac{2}{3},\frac{1}{3},0$) and ($\frac{1}{3},\frac{2}{3},0$) respectively. It is known that for these types of structures $10.l$ reflections are sufficient for the structure determination. Writing the summation for M and X atoms separately for an nH polytype having n X atoms and $n/2$ M atoms lying symmetrically between two alternate X atoms, we get

$$F_{10.l} = f_X \sum_{z_j=0,2}^{2n-2} \exp 2\pi i\left(x_j + \frac{lz_j}{2n}\right) + f_M \sum_{z_{j'}=1,5}^{2n-3} \exp 2\pi i\left(x_{j'} + \frac{lz_{j'}}{2n}\right), \qquad (1)$$

$I_{10.l} \propto |F|^2$.

The summation over the atoms has been replaced by a summation over the z coordinates of all atoms with the x coordinate taken as a function of z. x_j and $x_{j'}$ will be 0, $\frac{2}{3}$ or $\frac{1}{3}$ depending on whether the atom is at A (or α), B (or β), C (or γ) orientation for a certain value of z_j or $z_{j'}$. Since there are $3n/2$ atoms in an nH or nR polytype, there will be $3n/2$ terms in the structure-factor calculation: n terms in the X summation and $n/2$ terms in the M summation. Let us try to write the X summation in terms of the M summation. Take a structure MX_2 and write in ABC notation

$$\begin{array}{rl} & A\,\gamma B\;\; C\,\alpha B\;\; A\,\gamma B\;\; C\,\beta A\ldots \\ z_j = & 0\quad 2\;4\quad 6\;8\quad 10\;12\;14 \\ z_{j'} = & \quad 1\qquad 5\qquad 9\qquad 13. \end{array}$$

Any sandwich ($A\,\gamma B$) at some position in the sequence will have a $\gamma(M)$ atom at z with an A atom at $z-1$ and a B atom at $z+1$ respectively.

The contribution of this sandwich to the total summation for X atoms will be

$$\exp 2\pi i\left[0 + \frac{l(z-1)}{2n}\right] + \exp 2\pi i\left[\frac{2}{3} + \frac{l(z+1)}{2n}\right]$$

or

$$\exp 2\pi i\left[\frac{1}{3} + \frac{lz}{2n}\right]\left\{\exp\left[-2\pi i\left(\frac{1}{3} + \frac{l}{2n}\right)\right] + \exp\left[2\pi i\left(\frac{1}{3} + \frac{l}{2n}\right)\right]\right\}$$

or

$$\left[\exp 2\pi i\left(\frac{1}{3} + \frac{lz}{2n}\right)\right] \times 2\cos 2\pi\left(\frac{1}{3} + \frac{l}{2n}\right)\ldots. \qquad (2)$$

This is just the contribution of an M atom at γ orientation of this sandwich to the summation over all different M atoms, multiplied by $2\cos 2\pi\,(\frac{1}{3} + l/2n)$. Similarly, if the sandwich had been ($B\,\alpha\,C$) or ($C\,\beta\,A$), which may be called sandwiches in clockwise orientation, it can be seen that a similar expression for α or β with the same multiplying factor will appear.

Had it been ($B\,\gamma A$) instead of ($A\,\gamma B$), (2) would have been

$$2\cos 2\pi\left(-\frac{1}{3} + \frac{l}{2n}\right)\exp 2\pi i\left[\frac{1}{3} + \frac{lz}{2n}\right],$$

i.e. only the multiplying factor would change and it will be the same for ($C\,\alpha\,B$) and ($A\,\beta\,C$) sandwiches which may be called anticlockwise sandwiches.

Equation (1) can be written as

$$F_{10.l} = f_X(A_{\text{clock}} + A_{\text{anticlock}}) + f_M(B_{\text{clock}} + B_{\text{anticlock}}),$$

where the terms in parentheses are summations over the atoms in clockwise and anticlockwise sandwiches and are

$$A_c + A_a = \sum_{z_j = 0,2}^{2n-2} \exp 2\pi i\left(x_j + \frac{lz_j}{2n}\right)$$

and

$$B_c + B_a = \sum_{z_{j'}=1,5}^{2n-3} \exp 2\pi i\left(x_{j'} + \frac{lz_{j'}}{2n}\right).$$

Therefore,

$$F_{10.l} = f_X\left[2B_c \cos 2\pi\left(\frac{1}{3} + \frac{l}{2n}\right) + 2B_a \cos 2\pi\left(-\frac{1}{3} + \frac{l}{2n}\right)\right] + f_M(B_c + B_a)$$

$$= \left[2f_X \cos 2\pi\left(\frac{1}{3} + \frac{l}{2n}\right) + f_M\right]B_c + \left[2f_X \cos 2\pi\left(-\frac{1}{3} + \frac{l}{2n}\right) + f_M\right]B_a$$

or

$$F_{10.l} = \left[2f_X \cos 2\pi\left(\frac{1}{3} + \frac{l}{2n}\right) + f_M\right] \times \sum_{z_{j'c}=\text{clockwise}} \exp 2\pi i\left(x_{j'c} + \frac{lz_{j'c}}{2n}\right) + \left[2f_X \cos 2\pi\left(-\frac{1}{3} + \frac{l}{2n}\right) + f_M\right] \times \sum_{z_{j'a}=\text{anticlockwise}} \exp 2\pi i\left(x_{j'a} + \frac{lz_{j'a}}{2n}\right)$$

or

$$I_{10.l} \propto |F_{10.l}|^2.$$

The expression does not contain any term for the summation of X atoms. It has summation over M atoms only in clockwise and anticlockwise types of sandwiches and therefore the total length of the calculation will be one third of the original.

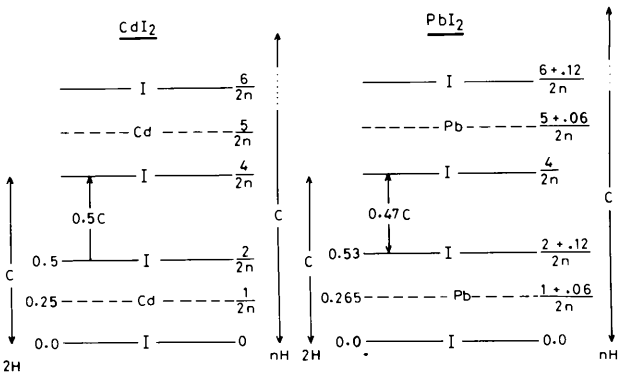

Fig. 1. Layer spacing in CdI_2 (or $CdBr_2$) and PbI_2.

The formula can be used for symmetric structures like CdI_2 or $CdBr_2$ as it is, but has to be modified for unsymmetric structures like PbI_2. In PbI_2 (Terpstra & Westenbrink, 1926) the spacing between the different sandwiches is not the same as the width of the sandwich itself (Fig. 1). Therefore, the summation over I has two types of terms, one half having the coordinates (x,y,z) like CdI_2 or $CdBr_2$ and the other half $(x, y, z + 2z')$ where z' is $0{\cdot}06/2n$. In the present case both these summations are replaced by the summation over Pb atoms represented by $(x, y, z + z')$. Therefore, if (3) is used for PbI_2, $z_{j'a}$ or $z_{j'c}$ should be replaced by $(z_{j'a} + 0{\cdot}06)$ or $(z_{j'c} + 0{\cdot}06)$ respectively.

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