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Geometrical Properties of MDO Polytypes and Procedures for Their Derivation. II. OD Families Containing OD Layers of $M > 1$ Kinds and Their MDO Polytypes

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Abstract

The condition for MDO polytypes formulated in paper I [Dornberger-Schiff (1982). *Acta Cryst.* A**38**, 483–491] is applied to OD structures containing OD layers of $M > 1$ kinds. Methods for ascertaining whether a certain polytype is an MDO polytype or not, and for deducing a complete list of MDO polytypes for any family of polytypes are given. These are applied to $YCl(OH)_2$ and some MeX_2 polytype families.

Introduction

Amongst the polytypic substances whose structures turn out to be OD structures consisting of OD layers of more than one kind, there are some of great theoretical and practical importance, such as the various phyllosilicates, pyroxenes, sulfides, selenides and others. Compilation of a complete list of MDO polytypes for such polytypic substances is of particular importance because this may lead to a recognition of the structure, even if no single crystals are available (see *e.g.* Weiss & Ďurovič, 1980).

The definition of MDO polytypes for polytypic substances has been given in paper I of this series (Dornberger-Schiff, 1982). This and other notions – such as τ and ρ operations – described there will also be used here. As already mentioned, layers of different kinds are to be given different superscripts. Four different categories of families of OD structures have been distinguished (Dornberger-Schiff, 1964; Grell & Dornberger-Schiff, 1982; Grell, 1980), of which category II contains only polar layers, with equivalent layers related exclusively by τ operations, so that no ρ

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operation links a layer to itself or to another layer, whereas in categories I, III and IV there are ρ operations linking layers either to themselves or to other layers.

The sequence of kinds of layers in any polytype of a family, without any indication of their relative position, has been given for the four categories as follows (Grell & Dornberger-Schiff, 1982).

Category I

$$\ldots A_1^1 b_2^2 \ldots b_M^M d_{M+1}^M d_{M+2}^{M-1} \ldots d_{2M-1}^2 A_{2M}^1 b_{2M+1}^2 \ldots$$

Category II

$$\ldots b_0^M b_1^1 b_2^2 \ldots b_M^M b_{M+1}^1 \ldots b_{2M}^M \ldots$$

Category III

$$\ldots d_0^1 b_1^1 b_2^2 \ldots b_M^M d_{M+1}^M \ldots d_{2M}^1 b_{2M+1}^1 \ldots$$

Category IV

$$\ldots d_0^2 A_1^1 b_2^2 \ldots b_{M-1}^{M-1} A_M^M d_{M+1}^{M-1} \ldots d_{2M-2}^2 A_{2M-1}^1 b_{2M}^2 \ldots.$$

In analogy to paper I, tests for ascertaining whether a given polytype is an MDO polytype or not are discussed in the following. After that, procedures for obtaining a complete list of all MDO polytypes of a given family are presented.

Before entering into these discussions, some useful tools simplifying this task are introduced, which are based on properties of polytypes with $M > 1$.

Some remarks on categories I, III and IV

A uniform treatment of the categories I, III and IV is made possible by regarding any non-polar layer A^1 and/or A^M as being composed of two half-layers d^1 and b^1 and/or b^M and d^M, respectively. The half-layers are then treated as if they were layers; only the subscripts of layers of categories I and IV have to be changed accordingly. The M-tuples of layers $b^1 b^2 \ldots b^M$ or $d^M d^{M-1} \ldots d^1$ are identical with the packets introduced by Ďurovič (1974); they contain layers of any kind exactly once.

Classes of *n*-tuples

Whereas in polytypes containing only equivalent OD layers all n-tuples of layers for a certain number n are of the same chemical composition, this is no longer the case for polytypes containing $M > 1$ kinds of layers. Therefore application of condition MDO(ii) is more complex for such polytypic families. For tackling this problem the variety of n-tuples is classified in the following way: Two finite sequences of OD layers $L_{r+1} L_{r+2} \ldots L_{r+m}$ and $L_{s+1} L_{s+2} \ldots L_{s+n}$ are regarded as belonging to the same class, if and only if $m = n$ and $L_{r+1}{:}\tau{:}L_{s+1}$ or $L_{r+1}{:}\rho{:}L_{s+n}$. This means that two finite sequences of OD layers belong to the same class if they are n-tuples with the same number n and either begin with equivalent layers lying the same side up, or one begins and the other ends with equivalent layers with equivalent sides of these layers facing up and down, respectively.

Remark: n-tuples of the same class need not necessarily be geometrically equivalent; if they are not, we call them of the same class but of different kind.

With the concept of classes we can say: condition MDO(ii) is violated by a polytype π_0, if and only if for at least one of the classes of n-tuples it is possible to construct a polytype π_1 containing only a selection of the kinds of n-tuples present in that class of polytype π_0.

Test for the MDO character of a polytype

Category II

In this category equivalence of n-tuples can only be brought about by τ operations. The existence of a total operation $L_x{:}\tau{:}L_{x+M}$ suffices to ensure that all n-tuples of the same class are equivalent, and thus that the polytype is an MDO polytype. This is also a necessary condition.

Category III

Categories I and IV are treated the same as category III. In the following, condition MDO(ii) is to be discussed for different classes of n-tuples in succession: first, for the class of M-tuples identical with packets (leading to condition A). Then for the class of $2.M$-tuples constituting pairs of packets (condition B) and for $n'.M$-tuples constituting n'-tuples of packets (condition C). Finally, another n-tuples of layers are to be treated.

Condition A: All packets of an MDO polytype are equivalent. (Any packet $b^1 \ldots b^M$ of a polytype containing equivalent packets will in the following be indicated by the letter p, any packet $d^M \ldots d^1$ by the letter q.)

Condition B: In any MDO polytype all packet pairs pq are equivalent, and so are all packet pairs qp.

Condition C: If π_1 is an MDO polytype, then there is no polytype π_0 of the polytype family in which the kinds of n'-tuples of consecutive packets for some number n' constitute only a selection of the kinds of packet n'-tuples contained in π_1.

If condition A is violated by a polytype π_0, *i.e.* not all packets are equivalent, then it is possible to construct a polytype π_1 containing only one of the kind of packets contained in π_0, *i.e.* this class of M-tuples is reduced

If condition B is violated, *i.e.* not all pairs pq and/or not all pairs qp are equivalent, a similar construction is possible, reducing the kinds of packet pairs without introducing any new kind of packet pair.

If conditions A, B and C hold for a polytype, then, referred to its packets considered as layers, it is either fully ordered or it is an OD structure consisting of equivalent layers (conditions A and B), and referred to its packets as layers, it is an MDO structure (condition C).

Polytypes for which conditions A, B and C hold will in the following be called P/MDO polytypes.

A test to show whether a certain polytype is a P/MDO polytype or not may thus be conducted along the line indicated in flow chart 1 (Fig 1): first it is ascertained whether conditions A and B hold. The test of condition C follows then, as described in Table 1 of part I. A P/MDO polytype may be an MDO polytype (referred to its layers) or only a P/MDO polytype. This depends on the question of whether there exists a class of n-tuples, not identical with any of the classes of packet n'-tuples, which violates condition MDO(ii) or not.

The polytypes of a family may thus be classified as MDO polytypes, only P/MDO polytypes (*i.e.* P/MDO polytypes which are not MDO polytypes) and not P/MDO polytypes, as indicated in Fig. 2.

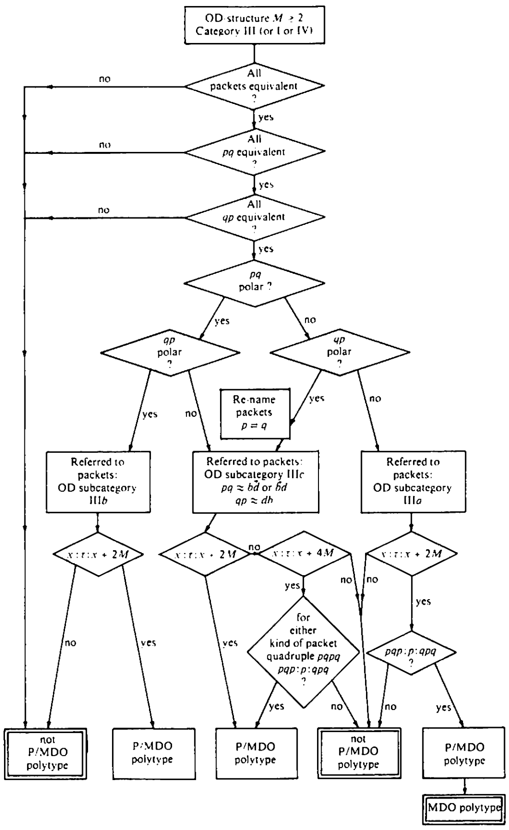

Fig. 1. Flow chart 1.

Distinction between only P/MDO polytypes and MDO polytypes

In order to test whether a P/MDO polytype is an MDO polytype or only a P/MDO polytype, we may conveniently distinguish between:

n-tuples lying entirely within a single packet, *i.e.* containing only layers b^j, or layers d^j;

n-tuples lying entirely within a packet pair, but not within a packet, *i.e.* either of the kind $d^r \ldots d^1 b^1 \ldots b^s$ or of the kind $b^r \ldots b^M d^M \ldots d^s$;

n-tuples of arbitrary length but containing layers of at least three packets.

n-tuples lying entirely within a packet and belonging to the same class are in any P/MDO polytype of the same kind. This follows from the equivalence of the packets. Such n-tuples cannot, therefore violate condition MDO(ii).

n-tuples containing layers of at least three packets and belonging to the same class may violate condition MDO(ii), if shorter m-tuples lying within a packet pair do the same, or – if referred to packets as layers – the polytype constitutes one of the 'exceptional cases' excluded in paper I from further discussion. Such exceptional cases seem to be rather rare as already mentioned in paper I. They are not to be discussed here.

n-tuples lying entirely within a packet pair but not within a single packet and belonging to the same class have the following peculiarity: within any packet pair qp there is exactly one n-tuple* of the class starting with d^r and ending with b^s. For any $r \le M$ and any $s \le M$: $r \ne s$, there are exactly two n-tuples ($n = r + s$) of the same class, namely that starting with d^r and ending with b^s and that starting with d^s and ending with b^r (Fig. 3 with $r = 1$; $s = 2$). A similar statement holds for any packet pair pq. Therefore a violation of MDO(ii) can only come from such a class ($r \ne s$), if the two ($r + s$)-tuples belonging to it are of different kind (Fig. 3a), although with the same packets in another kind of packet pair of the family they are both of one of these kinds (Fig. 3b). A packet pair containing at least one

* Any n-tuple lying within a packet pair is unequivocally characterized by its kind of first and last layer and will be indicated accordingly.

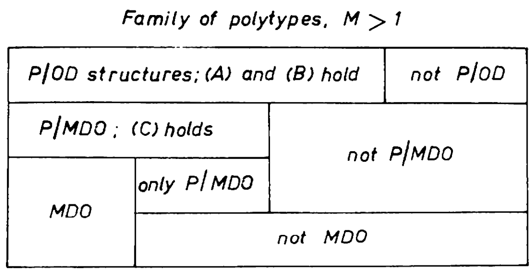

Fig. 2. Classification of polytypes of a family.

class of n-tuples violating condition MDO(ii) is, in the following, called a violating packet pair.

For ascertaining whether a packet pair qp is a violating packet pair it is convenient to distinguish between packet pairs according to their polarity or non-polarity and the polarity or non-polarity of the pair of adjacent ρ-equivalent layers $d^1 b^1$, as indicated in Table 1. The last column of Table 1 gives part of the solution to our question. Only the last line requires a special discussion. If the packet pair qp is polar, but $d^1 b^1$ is non-polar, there exists a non-polar part, *i.e.* a $2r$-tuple $d^r \ldots b^r$ (at least $d^1 b^1$), whereas $d^{r+1} \ldots b^{r+1}$ is polar, where $r < M$; this follows from the polarity of the packet pair.

The packet pair qp is not violating, if and only if one of the ρ operations converting $d^r \ldots b^r$ into itself also converts q into p; *i.e.* there exists an operation

$$d^r \ldots b^r : p : d^r \ldots b^r \leftrightarrow d^M \ldots b^r : p : d^r \ldots b^M$$

(see Fig. 4). In Fig. 3(a) there exists a ρ operation, the twofold axis converting d^1 into b^1 and *vice versa*, but q

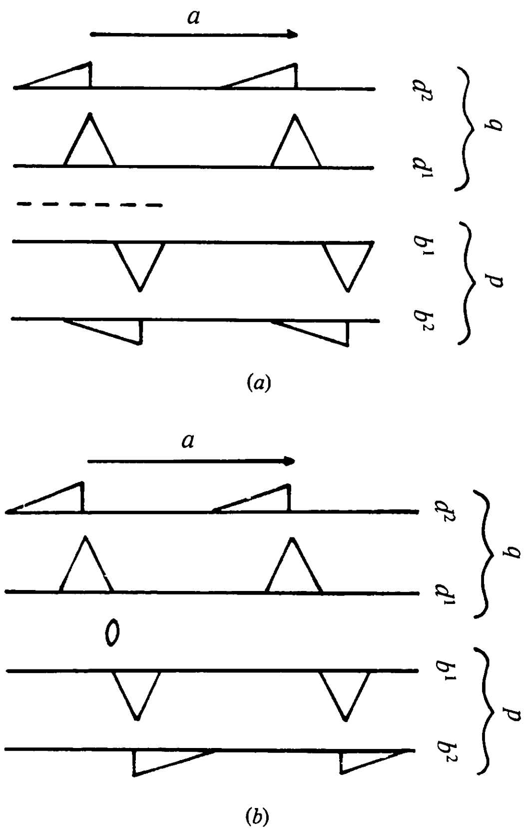

Fig. 3. Two different packet pairs qp containing the same kind of packet. (a) qp is polar, containing two kinds of layer triples $d^2 d^1 b^1$:no ρ:$d^1 b^1 b^2$. (b) qp is non-polar, containing only one kind of layer triple $d^2 d^1 b^1$:ρ:$d^1 b^1 b^2$, equivalent to $d^2 d^1 b^1$ of (a). Therefore the packet pair shown in (a) violates condition MDO(ii).

Table 1. *Polarity or non-polarity of the pair of adjacent ρ-equivalent layers $d^1 b^1$*

qp	$d^1 b^1$	Remark
non-polar	non-polar	not violating
non-polar	polar	cannot exist
polar	polar	not violating
polar	non-polar	possibly violating

is transformed into p by the glide plane which transforms d^1 into b^1 but not b^1 into d^1 and therefore the packet pair qp of Fig. 3(a) is a violating packet pair. Even if, in a certain polytype family, there is a non-polar packet pair qp (Fig. 5a), that does not mean that a polar packet pair must necessarily be a violating packet pair (Fig. 5b).

The procedure for ascertaining whether a packet pair violates condition MDO(ii) or not is summarized in flow chart 2 (Fig. 6).

A P/MDO polytype violates condition MDO(ii) and is thus an only P/MDO polytype, if qp and/or pq is a violating packet pair; a P/MDO polytype does not violate condition MDO(ii), and is thus an MDO polytype, if neither pq nor qp is a violating packet pair.

Examples

Yttrium hydroxy chloride, $YCl(OH)_2$

Two crystalline forms of this substance have been observed (Klevtsova & Klevtsov, 1965, 1966) and the relationships of their structures explained as OD structures of the same family, consisting of two kinds of non-polar OD layers (Dornberger-Schiff & Klevtsova, 1967; see also Grell & Dornberger-Schiff, 1982). If either of the two non-polar layers is replaced by polar halves, any polytype of this family appears to belong to

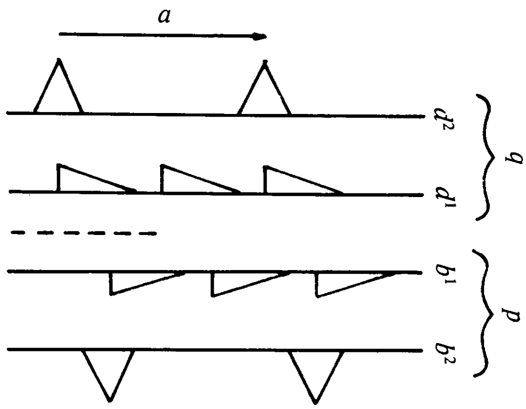

Fig. 4. A polar packet pair qp with non-polar layer pair $d^1 b^1$, and equivalent triples of layers with the equivalence resulting from $d^1 b^1$:ρ:$d^1 b^1 \leftrightarrow d^2 d^1 b^1$:$\rho$:$d^1 b^1 b^2$.

subcategory IIIa referred to packets $p = b^1 b^2$ and $q = d^2 d^1$. Proceeding as indicated above, the MDO character of the two observed crystalline forms may be tested:

Condition A: All packets are equivalent, because any packet consists of layer pairs $b^1 b^2$ or $d^2 b^1$ and these are equivalent according to the VC (vicinity condition).

Condition B: All packet pairs qp correspond to the sheets and are equivalent in any polytype of this family and thus also in the two crystalline forms. The packet pairs pq are different in the two crystalline forms but equivalent in either of them.

Condition C: Referred to packets, either of the crystalline forms belongs formally to subcategory IIIa, because qp is non-polar and so is pq in either of the two crystalline forms. The additional conditions for MDO polytypes of subcategory IIIa listed in Table 1 of paper I are fulfilled in either of the two crystalline forms. Either of them is thus a P/MDO polytype.

None of the packet pairs qp and pq in either of the crystalline forms violates the MDO condition, as all these packet pairs are non-polar. Either of the two crystalline forms is thus an MDO polytype.

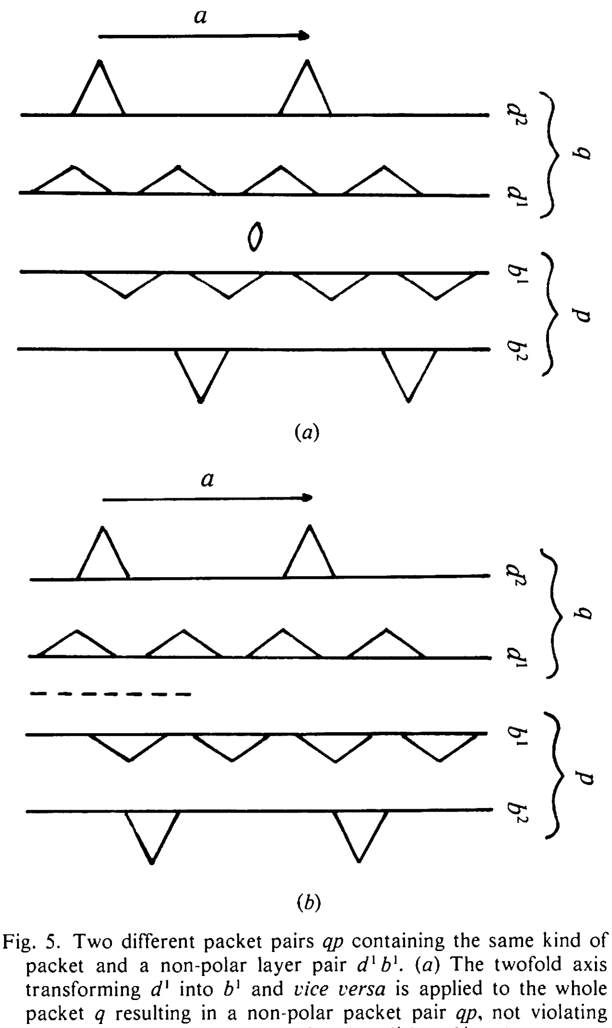

Fig. 5. Two different packet pairs qp containing the same kind of packet and a non-polar layer pair $d^1 b^1$. (a) The twofold axis transforming d^1 into b^1 and *vice versa* is applied to the whole packet q resulting in a non-polar packet pair qp, not violating MDO(ii). (b) The a glide transforming d^1 into b^1 and *vice versa* transforms d^2 into b^2 but not b^2 into d^2. Therefore the packet pair is polar but does not violate condition MDO(ii).

Further examples

The discussion of some frequently occurring polytypes of some MeX_2 substances containing simple hexagonal atomic planes is summarized in Table 2. It turns out that amongst them there are MDO polytypes, only P/MDO polytypes but also not-P/MDO polytypes (see column 10 of Table 2).

The Ramsdell symbols in column 3 are quoted as indicated by the respective authors and also in the book by Verma & Krishna (1966). The figure in any of these Ramsdell symbols for $TaSe_2$ and $NbSe_2$ gives the number of sandwiches (XMeX) per period, whereas for the other substances the number of anion planes (X) per period is indicated.

Any polytype is indicated by means of ABC notation giving the absolute position of atomic planes in column 4, and by generalized Hägg symbols in column 5, giving the displacement of any atomic plane relative to its predecessor with Me relative to X, and X relative to

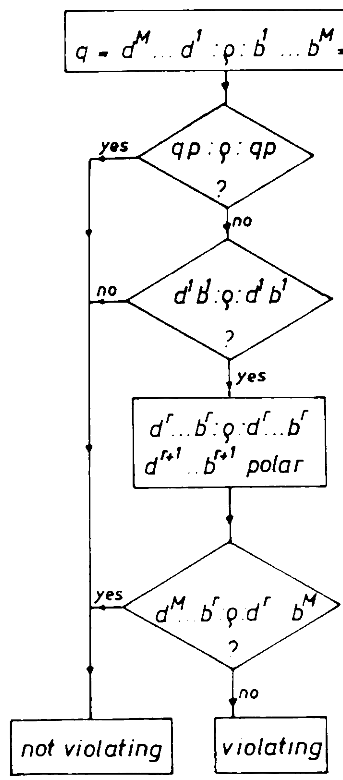

Fig. 6. Flow chart 2. Test of qp.

Me in the first line, and X relative to X in the second line.

These substances belong to category I with $M = 2$, the metal atoms Me constitute the non-polar layer A^1 to be split for our purpose into $d^1 b^1$, the anion planes X are polarized and thus polar and denoted by b^2 and d^2. The packets $X\mathrm{Me}_{1/2}$ and $\mathrm{Me}_{1/2}X$ are denoted by $d^2 d^1 = q$ and $b^1 b^2 = p$, respectively. The packet pairs $qp = X\mathrm{Me}X$ are thus the sandwiches, the packet pairs pq consist of the atomic planes $\mathrm{Me}_{1/2}XX\mathrm{Me}_{1/2}$. With these conventions, the substances belong formally to category III and the tests for their MDO character are to be taken accordingly. The main steps and results are indicated in Table 2.

Condition A: In any of the polytypes the packets are equivalent.

Condition B: Equivalence of packet pairs is indicated in columns 6 and 7. Only examples 1, 2, 3, 6 and 7 fulfil this condition and are to be tested further.

Condition C: Nos. 1, 3 and 6 belong to subcategory III*a*. For MDO polytypes belonging to this subcategory a total τ operation $L_x{:}\tau{:}L_{x+2}$ is required and the additional condition $b_1 d_2 b_3{:}\rho{:}d_2 b_3 d_4$ (*cf.* Table 1, paper I) must be fulfilled, *i.e.* in the case of packets $p_1 q_2 p_3{:}\rho{:}q_2 p_3 q_4$ must hold. In all these cases the additional condition is valid and the total τ operations are indicated in column 9 by T (translation) and c (c glide perpendicular to **b**), respectively. Nos. 2 and 7 belong to subcategory III*c*. As follows from Table 1 of paper I the existence of a total τ operation $L_x{:}\tau{:}L_{x+2}$ suffices to ensure the MDO character for polytypes of this subcategory, this is a c glide perpendicular to **b** for No. 2 and a translation for No. 7. Result: all the quoted examples fulfil condition C and are therefore P/MDO polytypes.

In order to distinguish between MDO and only P/MDO polytypes the packet pairs have to be classified as violating or non-violating. The layer pair $d^1 b^1$ is non-polar, and so is the pair $b^2 d^2$. The two occurring kinds of packet pairs qp (sandwiches) are non-polar and thus non-violating. The polarity of packet pairs pq is indicated in column 8. Polar packet pairs are violating. the result of this discussion is given in column 10.

Procedure for obtaining all MDO polytypes of a family

For obtaining all MDO polytypes of a family the properties A, B, and C will be used.

The MDO conditions do not impose any limitation on the kind of packet present in an MDO polytype, so that, in order to obtain all MDO polytypes, all kinds of packets which may occur in the family have to be considered. If the family is characterized by a representative part, *i.e.* a part of a polytype containing layer pairs of all those kinds which occur in polytypes of the family (Grell & Dornberger-Schiff, 1982), all kinds of packets may be obtained in the following way. Starting with the first pair $b^1 b^2$ of the packet contained in the representative part, all positions of b^3 leading to a layer pair $b^2 b^3$ equivalent to the corresponding pair of the representative part are considered. They are related to one another by τ operations converting b^2 into itself. Starting with any of the triples of different kind thus obtained (of equivalent triples only one need be considered), all quadruples $b^1 b^2 b^3 b^4$ are obtained by adding b^4 in all those ways leading to layer pairs $b^3 b^4$ of the kind indicated in the representative part. Proceeding in a similar way, quintuples ..., M-tuples = packets result.

For category II the $(M+1)$-tuples $b_1^1 b_2^2 \ldots b_M^M b_{M+1}^1$ are then obtained for any kind of packet in a strictly

Table 2. *Some frequently occurring polytypes of* Me X_2 *substances and their OD character*

1	2	3	4	5	6	7	8	9	10
No.	Substance	Ramsdell symbol	ABC notation	Generalized Hägg symbol	qp equivalent	pq equivalent	pq non-polar	Operation	Result
1	CdI_2	$2H$	$A\gamma B$	$\|{-}{-}_{-}\|$	+	+	+	T	MDO
2	$CdBr_2$, PbI_2	$4H$	$A\gamma B\ C\alpha B$	$\|{-}{-}_{+}{+}{+}_{-}\|$	+	+	–	c	only P/MDO
3	$CdBr_2$, PbI_2	$6R$	$A\gamma B\ C\beta A\ B\alpha C$	$\|{-}{-}_{+}\|_{3}$	+	+	+	T	MDO
4	$CdBr_2$	$6H$	$A\gamma B\ C\beta A\ C\alpha B$	$\|{-}{-}_{+}{-}{-}_{-}{+}{+}_{-}\|$	+	–			not P/MDO
5	PbI_2	$6H$	$A\gamma B\ C\alpha B\ A\gamma B$	$\|{-}{-}_{+}{+}{+}_{-}{-}{-}_{-}\|$	+	–			not P/MDO
6	$TaSe_2$, $NbSe_2$	$2H$	$A\gamma A\ B\gamma B$	$\|{-}{+}_{+}{+}{-}_{-}\|$	+	+	+	c	MDO
7	$NbSe_2$, MoS_2	$3R$	$A\beta A\ B\gamma B\ C\alpha C$	$\|{+}{-}_{+}\|_{3}$	+	+	–	T	only P/MDO
8	$TaSe_2$	$4H$	$A\gamma B\ A\gamma A\ B\gamma A\ B\gamma B$	$\|{-}{-}_{-}{-}{+}_{+}{+}{+}_{+}{+}{-}_{-}\|$	–	–			not P/MDO
9	$NbSe_2$	$4H$	$A\beta A\ B\gamma B\ A\beta A\ C\beta C$	$\|{+}{-}_{+}{+}{-}_{-}{+}{-}_{-}{-}{+}_{+}\|$	+	–			not P/MDO

analogous way. For any of the $(M+1)$-tuples, any of the operations

$$b_1^1:\tau^{(j)}:b_{M+1}^1$$

applied to all layers leads to an MDO polytype, and all MDO polytypes are included in the list thus obtained.

For category III the $(M+1)$-tuples $b^1 b^2 \ldots b^M d^M$ and $d^1 b^1 \ldots b^M$ are obtained in a similar way for any kind of packet. Take note that two equivalent layer pairs $d^{1(j)} b^1$ resulting from different positions $d^{1(j)}$ of the layer d^1 are related either by a τ or by a ρ operation, if the layer pair is polar, or by both, if the layer pair is non-polar. A similar statement applies for the different positions of d^M. The packet pairs qp and pq which may occur in any MDO polytype have then to be found. Any of them must necessarily contain equivalent, *i.e.* ρ-equivalent packets. To any kind of $(M+1)$-tuple $d^1 p$ all packet pairs qp containing it and consisting of equivalent packets result from the application of the ρ operations converting b^1 into d^1. If the layer pair $d^1 b^1$ is polar, then all resulting packet pairs are non-violating. If $d^1 b^1$ is non-polar, then the ρ operations converting $d^1 b^1$ into itself lead to non-violating packet pairs, and those converting only b^1 into d^1 and not d^1 into b^1 lead to violating packet pairs.

In a similar manner, all non-violating and violating packet pairs pq result.

In order to obtain a complete list of all MDO polytypes (or P/MDO polytypes) all combinations of non-violating packet pairs pq and qp containing the same kind of packet (or those of all packet pairs pq and qp containing the same kind of packet excluding those combinations which are already obtained) have to be considered. For any combination the polarity or non-polarity of the packet pairs qp and pq have to be ascertained. The packets are now to be treated as if they were equivalent layers and the procedure of Table 2 of paper I for the respective subcategories III*a*, III*b* or III*c* is to be applied to any combination of packet pairs.

Example

We may now deduce all MDO and only P/MDO polytypes for MeX_2 families consisting of simple hexagonal atomic planes, in accordance with the described procedure. For this purpose we use the generalized Hägg symbols described above. The possible kinds of packet pairs are indicated in Table 3.

The combination of either of the two pairs qp with either of the two non-polar, non-violating pairs pq (Table 4*a*) leads to one kind of packet triple qpq each, and also to one kind of packet quadruple each, and any of these to one MDO polytype, by application of the $L_x:\tau:L_{x+2}$ operations. Because pq is non-polar and so is qp, these polytypes belong – referred to packets – to subcategory III*a*, and the described procedure leads – corresponding to Table 2 of paper I – to a complete list of all MDO polytypes.

The combination of the violating packet pair pq (3) with either of the kinds of pairs qp (I) and (II) (Table 4*b*) leads to one triple pqp each, any of these corresponds to a triple $b^{\rightarrow}d\ b$, *i.e.* to category III*c*, and

Table 3. *Possible kinds of packet pairs in* MeX_2 *polytypes*

qp	pq non-violating	pq violating
(I) $++\equiv--$	(1) $+_{+}+\equiv-_{-}-$	(3) $+_{+}-\equiv-_{-}+\equiv+_{-}-\equiv-_{+}+$
(II) $+-\equiv-+$	(2) $+_{-}+\equiv-_{+}-$	

Table 4. *Deduction of the MDO and only P/MDO polytypes for the* MeX_2 *families from the combination of the kinds of packet pairs*

(*a*) Combination of either of qp with either of non-violating pq

Packet pairs	qpq	$qpqp$	MDO	No. (Table 2)
(I) (1)	$++_{+}++$	$++_{+}++_{+}$	$\lvert ++_{+}\rvert\equiv\lvert --_{-}\rvert$	1
(I) (2)	$++_{-}++$	$++_{-}++_{-}$	$\lvert ++_{-}\rvert\equiv\lvert --_{+}\rvert$	3
(II) (1)	$+-_{-}-+$	$+-_{-}-+_{+}$	$\lvert +-_{-}-+_{+}\rvert\equiv\lvert -+_{+}+-_{-}\rvert$	6
(II) (2)	$+-_{+}-+$	$+-_{+}-+_{-}$	$\lvert +-_{+}-+_{-}\rvert\equiv\lvert -+_{-}+-_{+}\rvert$	–

(*b*) Combination of pq (3) with either of qp

Packet pairs	pqp	$pqpq$ $b^{\rightarrow}d\,b^{\rightarrow}d$	$pqpq$ $b^{\rightarrow}d\,b^{\leftarrow}d$	only P/MDO	No. (Table 2)
(3) (I)	$+_{+}--$	$+_{+}--_{-}+$		$\lvert +_{+}--_{-}+\rvert\equiv\lvert --_{+}++_{-}\rvert$	2
			$+_{+}--_{+}+$	$\lvert +_{+}--_{+}+\rvert$	–
(3) (II)	$+_{+}-+$	$+_{+}-+_{+}-$		$\lvert +_{+}-\rvert\equiv\lvert +-_{+}\rvert$	7
			$+_{+}-+_{-}-$	$\lvert +_{+}-+_{-}-\rvert$	–

the respective procedure is to be applied. For either of the triples, one kind of quadruple corresponding to $b^{\rightarrow}d\ b^{\rightarrow}d$ and one kind of quadruple corresponding to $b^{\rightarrow}d\ b^{\leftarrow}d$ result, each leading to one only P/MDO polytype with $m = 2$ and $m = 4$, respectively.

It is remarkable that only three of the four MDO polytypes are amongst the frequently occurring polytypes listed in Table 2, but also two of the four only P/MDO polytypes (namely those with $m = 2$).

Concluding remarks

Although classification of polytypes of any family as MDO, only P/MDO or not P/MDO and deduction of all MDO polytypes and all only P/MDO polytypes is not too difficult, the explanation of the corresponding procedures may seem fairly involved. The reason is that by far the most OD crystals contain layers of not more than two different kinds, and for such families there is obviously only one kind of packet. Furthermore, by far the most OD crystals with $M > 1$ belong to category IV or category I – and treated as category III – there is thus only one position of d^1 relative to b^1 and for category IV also only one position of d^M relative to b^M, namely those leading together with b^1 or b^M to A^1 and A^M, respectively.

Although, as exemplified in Table 2, MDO and only P/MDO polytypes are not the only polytypes occurring in nature, they certainly seem to occur more frequently than others. In a number of polytype families they are indeed the only polytypes so far observed. Their knowledge may help for identifying the polytypes present (or mainly present) in a sample consisting of a multitude of crystals too small for single-crystal work, from powder diffraction diagrams. In this way they have already been used for the identification of vermiculite polytypes (Weiss & Ďurovič, 1980; Weiss, 1976).

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Dynamic Structure Factors for Excitations in Modulated Structures

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Abstract

A phenomenological Landau theory yields new excitations in incommensurate structures corresponding to a phase and amplitude fluctuation of the modulating function. The dynamic structure factors for the new excitation modes are calculated in harmonic approximation and the influence of phase and amplitude fluctuations is discussed.

1. Introduction

In recent years structures with a static periodical displacement of the atoms from their perfect lattice

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