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POLYTYPISM OF MICAS: OD-INTERPRETATION, STACKING SYMBOLS, SYMMETRY RELATIONS

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Abstract—From the symmetry point of view, micas may be classified as follows: those with all three octahedrally coordinated sites occupied by the same cation (homo-octahedral micas), those with only two of these sites occupied by the same cation (meso-octahedral micas), and those with the three sites occupied by different cations or by two different cations and a void, in an ordered manner (hetero-octahedral micas). For any of these three classes, mica polytypes, idealized in accordance with the generalized Pauling model, can be interpreted as OD structures consisting of octahedral OD layering and tetrahedral OD layering in which an interlayer cation plane is sandwiched between tetrahedral sheets. A mica layer built up by an octahedral sheet and two halves of tetrahedral sheets on either side consists of two OD packets linked by a two-fold rotation.

The orientation of any OD packet may be given by a number from 0 to 5 (related to a hexagonal coordinate system). A dot behind or before these numbers is used to denote the position of the octahedral layer (number + dot = orientational character). The displacement of a packet against its predecessor is characterized by a vector from the origin of a packet p_n (or q_{n-1}) to the origin of the adjacent packet p_{n+1} (or p_{2n}). These displacements may also be symbolized by numbers from 0 to 5 (displacement characters); a zero displacement is symbolized by *. Any mica polytype (ordered or disordered) can thus be described by a two-line symbol. The orientational characters are located on the first line, and the displacement characters on the second. Any symbol, therefore denotes unequivocally the stacking layers in a polytype. The space-group symmetry of ordered polytypes follows directly from the symbol.

Key Words—Mica, Order-disorder, Polytypism, Stacking symbol, Symmetry.

INTRODUCTION

Using the Pauling (1930) model of mica, Hendricks and Jefferson (1939) interpreted the Weissenberg diagrams of more than 100 specimens and found that all modifications may be referred to unit cells which are multiples of the same subcell, having symmetry Cm. Pabst (1955) showed that the space group of this subcell is $C2/m$. Smith and Yoder (1956) derived their well known symbolism of mica polytypes on the basis of a single ideal mica layer with the symmetry C12/m(1). Also Ross *et al.* (1966) based their vector stacking symbolism for characterizing mica polytypes on a centrosymmetrical mica layer, with the same symmetry. Likewise, Zvyagin (1964) based his deduction of the regular mica polytypes on the same assumption, but he used the tetrahedral and octahedral networks as separate building units. For the trioctahedral case the possibilities deduced by Smith and Yoder resulted. For the dioctahedral case Zvyagin discussed on centrosymmetrical 2:1 layers.

Güven and Burnham (1967) found a dioctahedral mica with a non-centrosymmetrical 2:1 layer, namely a $3T$ muscovite with the symmetry C12(1) of the single layer. Zvyagin and Soboleva (1974) also described dioctahedral micas with non-centrosymmetrical 2:1 layers, found by electron diffraction.

From electron microscopic investigations of etch pits on lepidolite and zinnwaldite crystals, Brauer (1971) obtained strong indications of ordered occupation of the octahedral sites by three different cations. The contours of some single etch pits, due to stepwise etching, showed no symmetry, but were related to neighboring contours by a mirror plane. This effect is to be expected if the three octahedral sites per unit cell are occupied by three different chemical entities (different cations or a void) in an ordered way and if consecutive mica layers are related by a symmetry plane. From an ordering of the octahedral cations, C2 symmetry for the single layer would result. The existence of layers in phyllosilicates with ordered occupation of the octahedral positions by three different chemical entities was predicted by Dornberger-Schiff and Ďurovič (1975a, 1975b) and confirmed by the X-ray diffraction analysis of a $1M$ zinnwaldite by Guggenheim and Bailey (1977) and of a $3T$ lepidolite by Brown (1978).

The present paper is part of a program aimed at an OD interpretation[3] of polytypism in various classes of

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[3] An outline of this concept is given in the Appendix to a paper on kaolinites by Dornberger-Schiff and Ďurovič (1975a). See also Dornberger-Schiff (1979). The letters OD are derived from order-disorder, but OD phenomena should not be confused with order-disorder phenomena in alloys.

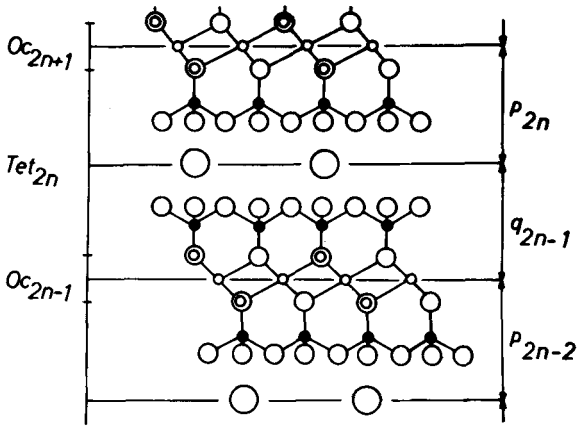

Figure 1. Projection along b of part of a mica structure; on the left: sequence of OD layers indicated; on the right: sequence of OD packets indicated. Large circle = interlayer cation; small circle = octahedral ion; medium circle = oxygen ion; double circle = OH.

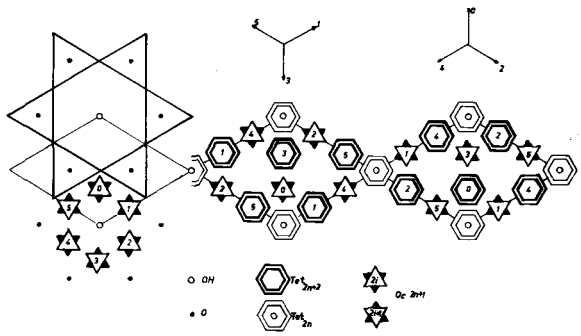

Figure 2. Left: tetrahedral layer with apical oxygens marked and the six possible positions of the octahedral layer numbered (0 to 5). Center and right: the six possible positions of $Oc_{2n,3}$ relative to the assumed position of T_{2n} and the six possible positions of T_{2n+2} relative to the latter. At the top: the possible layer to layer displacements and the numerical characters indicating them.

phyllosilicates, the description of their structures on a common basis, and the derivation of the respective sets of MDO polytypes defined by the so-called MDO conditions (i.e., simple or regular polytypes). Mica structures are treated on the basis of a generalized Pauling model. The silicate sheets are assumed to have hexagonal symmetry P(6)mm (without distinguishing between Si and Al), but the possiblity is considered that different octahedral cations may occupy the different sites in an ordered manner, with the translations a , a kept unchanged.

An OD interpretation of the mica structure is given below together with a symbolism for the representation of mica polytypes, and the symmetry relations following from any symbol.

TERMINOLOGY

The terms used are in accordance with the recommendations of the AIPEA Commission on Nomenclature. Orientational and displacement characters and their notations were introduced earlier (Dornberger-Schiff and Ďurovič, 1975a, 1975b) and the reader is referred to these papers for their meaning.

The crystallochemical discussion of the mica structures led to the well-known classification as di- and trioctahedral micas. This does not suffice for a geometrical characterization of the octahedral sheets, because it does not indicate the equivalence or non-equivalence of the occupation of the octahedral sites. Ďurovič and Mikloš (in preparation) considered the following types of site occupancy: (1) All octahedral sites are occupied by the same kind of chemical entity—homo-octahedral micas; (2) two octahedral sites are occupied by the same chemical entity, the third by a different entity, in an ordered way—meso-octahedral micas; (3) all three sites are occupied by three different chemical entities in an ordered way—hetero-octahedral micas. Thus, e.g., trioctahedral micas with three cations of the same element or a statistical distribution of different cations are called homo-octahedral micas; dioctahedral micas with two cations of the same element or a statistical distribution of different cations over two sites and a void or a cation of a different kind are called meso-octahedral micas.

In all types, the translations a_1, a_2 (related to a hexagonal coordinate system) common to the silicate sheet and the interlayer cations are assumed to be translations of the octahedral cations, if statistically disordered cations are treated as average cations.

OD INTERPRETATION OF THE MICA STRUCTURE

The description of mica polytypes as different stackings of mica layers or unit layers (Takeda and Sadanaga, 1969) does not deduce the stacking possibilities from any general principle. This is the aim of an OD interpretation which presupposes that any polytype of a given polytypic substance may be considered as consisting of parts periodic in two dimensions called OD layers, for which the vicinity condition (VC) holds. For micas these parts are of two kinds: octahedral OD layers (Oc) and tetrahedral OD layers (Tet). An octahedral OD layer consists of a plane of octahedrally coordinated cations and halves of the coordinating oxygen atoms on either side of the cation plane. A tetrahedral OD layer consists of an interlayer plane of cations and the two tetrahedral sheets adjacent to it, excluding the halves of oxygen atoms belonging to the octahedral OD layer (Figure 1). Such OD layers may be designated . . . L_0, L_1, L_2, . . . according to their sequence in the structure, with tetrahedral OD layers indicated by L_{2n}, and octahedral OD layers by L_{2n+1}. Tetrahedral and octahedral OD layers are designated Tet_{2n} and Oc_{2n+1}, respectively. All pairs of adjacent OD layers, i.e., (Tet_{2n}, Oc_{2n+1}) and (Oc_{2n-1}, Tet_{2n}), are geometrically equiva-

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lent in any homo-octahedral mica, and the same holds for any meso- and for any hetero-octahedral mica. The term OD layer implying the validity of the vicinity condition (see Appendix to Dornberger-Schiff and Ďurovič, 1975a and Dornberger-Schiff, 1979) is therefore justified for them. OD layers are sometimes called "layers" in the following discussion. The possible positions of the octahedral layer (Oc_{2n+1}) and tetrahedral layer (Tet_{2n+2}) relative to a fixed position of Tet_{2n} are shown in Figure 2.

The layer group of any tetrahedral layer is assumed to be P(6/m)mm with a statistical distribution of Si and Al atoms in the tetrahedral positions. Thus, a tetrahedral layer is indicated in Figure 2 by a regular hexagon.

In a homo-octahedral mica either the three octahedral positions marked 0, 2, 4 or those marked 1, 3, 5 are occupied (Figure 2). Three trigonal stars per unit cell with their centers at the octahedral sites represent the octahedral layer (Figures 2 and 3a). The octahedral ions and the coordinating oxygen atoms are arranged translationally equivalent with a translation $b/3 = (a_1 - a_2)/3$. The translational group for an octahedral layer is thus generated by $b_3/3$ and a_1 or a_2. Analogous to the nomenclature for space groups, the resulting Bravais net may be labelled by the Bravais symbol H, so that the layer group of an octahedral layer of a homo-octahedral mica is $H(\bar{3})1m$.

In meso-octahedral mica only two of the three octahedral sites are occupied by the same kind of cation. Thus, the octahedral layer has the symmetry P(3̄)1m and may be considered as represented by a trigonal star with its center at a vacant (or uniquely occupied) octahedral site (Figure 3b).

In a hetero-octahedral mica the three octahedral sites are occupied by three different chemical entities. The symmetry of the octahedral layer is P(3)12. Three different trigonal stars indicate the positions of the octahedral sites (Figure 3c), any one of which represents the symmetry of the layer.

For any mica, homo-, meso-, or hetero-octahedral, the layer pair (Oc_{2n+1}, Tet_{2n+2}) is related to (Tet_{2n}, Oc_{2n+1}) by a rotation around one of the two-fold axes of Oc_{2n+1}; thus these pairs are congruent.

Origin of OD layers

The origin of any OD layer has to be chosen according to convention for its layer group. For Tet_{2n} the origin is at a point with site symmetry 6/mmm, and as there is only one point per unit cell with this symmetry, the choice is unequivocal (except for the trivial ambiguity due to the translational group). The origin of an octahedral layer must be taken at a point with site symmetry 312, 31m or 3̄1m, in hetero-, meso-, and homo-octahedral mica, respectively.

In a meso-octahedral layer Oc_{2n+1} only one point per unit cell has this site symmetry—the unoccupied octahedral site (or the site occupied by a cation different from the other two octahedral cations) (Figure 3b). This site must therefore be selected as the origin. For a hetero-octahedral mica, the origin of a particular octahedral layer (e.g., Oc_1) may be arbitrarily chosen at one of the three octahedral sites. The origin of any other octahedral site is then unequivocally determined by the condition that the origin of all octahedral layers should be occupied by the same chemical entity. In a homo-octahedral layer Oc_{2n+1} any of the three octahedral sites could be selected as the origin (not depending on the choice of origin in any other layer).

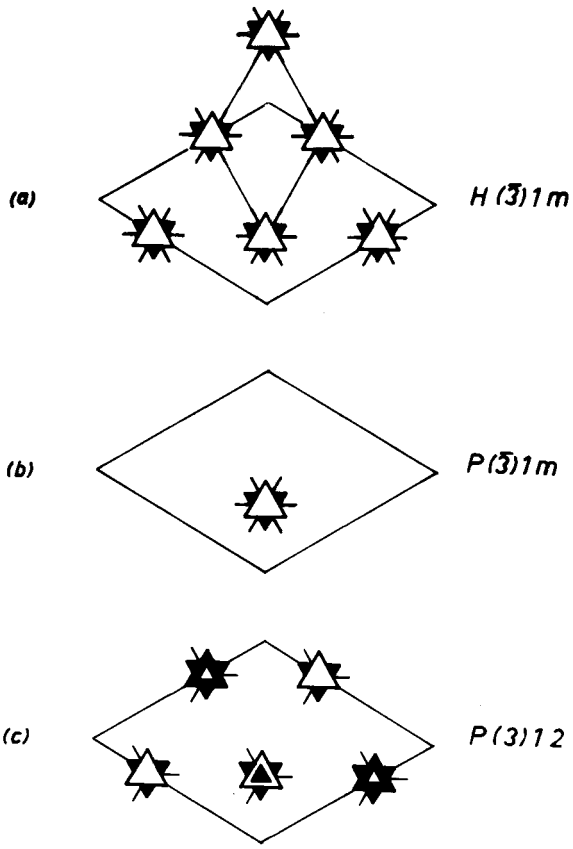

Figure 3. Schematic representation of an octahedral layer Oc_{2n+1}. (a) homo-octahedral; (b) meso-octahedral; (c) hetero-octahedral.

Structure and symmetry of OD layers

The layer group of either of the kinds of OD layers is nonpolar in all three classes of mica. Thus, the groupoid families[4] belong to category IV (Dornberger-

[4] The symmetry relations within any polytype are given by a set of coincidence operations; such a set has not the property of a group (in the mathematical sense) but of a groupoid, and is called an OD groupoid. The set of OD groupoids corresponding to a family of OD structures (e.g., the different mica structures) is called an OD groupoid family (see e.g., Dornberger-Schiff and Grell-Niemann, 1961).

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Table 1. Idealized atomic coordinates in OD layers referred to the origin of the respective layer and hexagonal basic vectors a_1, a_2, c_0.

	Atom[1]	Coordinates[2] x	y	z
Tetrahedral layer	K	0	0	0
	O_{bas}	1/2	0	z_{bas}
	Si, Al	1/3	2/3	z_{Si}
	$O_{1/2}$ H	0	0	z_{ap}
	$O_{1/2\ ap}$	1/3	2/3	z_{ap}
Hetero-octahedral layer	Ma	0	0	0
	Me	1/3	2/3	0
	Mi	2/3	1/3	0
	$O_{1/2}$	0	2/3	$(1 - z_{ap})$
Meso-octahedral layer	Ma	1/3	2/3	0
	$O_{1/2}$	0	2/3	$(1 - z_{ap})$
Homo-octahedral layer	Ma	0	0	0
	$O_{1/2}$	0	2/3	$(1 - z_{ap})$

[a] Ma, Me, and Mi indicate octahedral cations of different elements.
[2] bas = basal, ap = apical.

Schiff, 1975, 1979) and are indicated by the symbols of the two layer groups given in the first line, and by one of the possible displacements indicated by its components in the directions a_3, b_3 in the second line, below the interval between the layer groups (Grell-Niemann and Dornberger-Schiff, submitted for publication). In any of the three classes of mica polytypes, one of the possible displacements (i.e., projection of the vector from the origin of L_m to that of L_{m+1}), is $a_3/3$, so that the following symbols of OD groupoid families result:

	OD groupoid family	
Homo-octahedral mica	P(6/m)mm	H($\bar{3}$)1m
	[1/3, 0]	
Meso-octahedral mica	P(6/m)mm	P($\bar{3}$)1m
	[1/3, 0]	
Hetero-octahedral mica	P(6/m)mm	P(3)12
	[1/3, 0]	

The atomic positions within any OD layer are given in Table 1.

STACKING OF LAYERS IN MICA POLYTYPES AND DESCRIPTIVE SYMBOLS

The stacking of layers may be characterized by a vector leading from the origin of layer L_m to the origin of L_{m+1}, where the origin of any layer is chosen as indicated above. The normal projection of this vector onto the a_1-a_2 plane is called the displacement of L_{m+1} relative to L_m. In the mica structures, only the six displacements $\pm a_i/3$ (with i = 1, 2, 3) may occur as displacements from one layer to the next. For these displacements the numbers 0 to 5 are to be used as characters (see Figure 2 and Table 2).

Table 2. Vectors ⟨j⟩ indicated by the characters j and their sums.

j	⟨j⟩	j	⟨j⟩	
0	$a_3/3$	4	$a_1/3$	⟨j⟩ + ⟨j + 2⟩ =
1	$-a_1/3$	5	$-a_2/3$	⟨j + 1⟩
2	$a_2/3$	*	0	⟨j⟩ + ⟨j + 3⟩ = ⟨*⟩
3	$-a_3/3$			⟨j⟩ = ⟨j ± 6⟩

For *meso-octahedral micas* the stacking of layers in unequivocally characterized by the displacements of Oc_{2n+1} relative to Tet_{2n} and the displacements of Tet_{2n+2} relative to Oc_{2n+1}, or the characters of these displacements. A sequence of these characters can be used as a polytype symbol, as follows:

$$\text{i.j k.l} \ldots, \qquad (1)$$

where i, j, k, l are characters indicating the layer to layer displacements and the dots mark the positions of the octahedral layer. The two characters immediately behind and in front of a dot refer to layer pairs sharing an octahedral layer and must be either both even or both odd (parity condition). The orientation of the layers need not be indicated: All layers Tet_{2n} have the same orientation, and the orientation of any Oc_{2n+1} follows from the displacement of Oc_{2n+1} relative to Tet_{2n}.

In *hetero-octahedral micas* the displacement of Oc_{2n+1} relative to Tet_{2n} does not indicate unequivocally the orientation of Oc_{2n+1}. It indicates only the position of the octahedral site occupied by the cation used to fix the origin, but does not answer the question which of the other octahedral cations occupies which of the remaining sites. A prime or double prime replacing any dot in the symbol of form (1) is used to remove this ambiguity: Any character consisting of a number with a prime immediately in front or behind it indicates a right-handed octahedral layer; correspondingly, any character with a double prime indicates a left-handed octahedral layer.

In *homo-octahedral micas* the stacking of the layers is characterized by the displacements of Tet_{2n+2} relative to Tet_{2n}, while the position of the layer Oc_{2n+1} is unambiguously fixed by the position of the adjacent tetrahedral layers (see above). Thus, a symbol for a homo-octahedral mica can be written as a sequence of displacement characters

$$\text{r t s} \ldots, \qquad (2)$$

where r, t, s stand for numbers 0 to 5, indicating the vectors $\pm a_i/3$ (Figure 2 and Table 2). They indicate the displacement of a tetrahedral layer relative to the preceding tetrahedral layer, in contrast to the other two cases discussed above.

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The symbol for a periodic polytype consists of the sequence of characters referring to one period, placed between vertical bars.

POLYTYPE SYMBOLS REFERRING TO OD PACKETS

In many materials (e.g., kaolinite-type minerals) it is useful to introduce "OD packets" which, according to Ďurovič (1974), constitute the smallest continuous part, periodic in two dimensions which represents fully the chemical composition of a polytype. Any mica packet consists of half of a tetrahedral plus half of an octahedral layer (see Figure 1). From the fact that in any of the three types of mica the pairs of adjacent OD layers are equivalent, it follows that all packets are equivalent. Packets are polar and lie with one side or the other alternately facing up; they will be indicated by the letters p and q, as follows: $p_{2n} = Tet_{2n}/2 + Oc_{2n+1}/2$ and $q_{2n-1} = Oc_{2n-1}/2 + Tet_{2n}/2$. The origin of any packet will be taken at a hexad of its tetrahedral half layer.

The packets of the homo-, meso-, and hetero-octahedral micas have the layer groups P(3)1m, P1m(1), and P(1), respectively, and can be represented as shown in Figure 4(c), (b), and (a), respectively. The origin of any packet is at the center of the equilateral triangle (homo-octahedral) or at the point of the arrow (meso- and hetero-octahedral packet).

Orientation of the packets

In a *meso-octahedral mica* the orientation of any packet p_{2n} is unequivocally indicated by the displacement of Oc_{2n+1} relative to Tet_{2n}; that of any q_{2n-1} by the displacement of Tet_{2n} relative to Oc_{2n-1}. The numbers 0 to 5 introduced above are also used to denote these displacements. A packet pair (p, q) corresponds roughly to the 2:1 layer (with the addition of one half of an interlayer on either side). To distinguish between the orientation of packets lying with different sides up, a dot is placed between the numbers referring to p_{2n} and q_{2n+1}, thus marking the position of the octahedral layer. The orientation of any packet B_m (=p_m or q_m) is thus fully characterized by a number T_m and a dot to its right for m = 2n, or left for m = 2n + 1. Such a number followed or preceded by a dot is the orientational character of the respective packet. Within a symbol only one dot is given between the numerical parts of orientational characters referring to a packet pair corresponding to a 2:1 layer (see Figure 4b).

In a *hetero-octahedral mica* the left- or right-handedness (enantiomorphous nature) of a packet has also to be indicated. A certain packet (called a right-handed) and any packet congruent to it is indicated by a prime immediately before or after the number T_m referring to it; any packet enantiomorphous to it, by a double prime. In any packet pair p_{2n}, q_{2n+1} (containing a mica layer) the packets p_{2n} and q_{2n+1} are linked by a two-fold

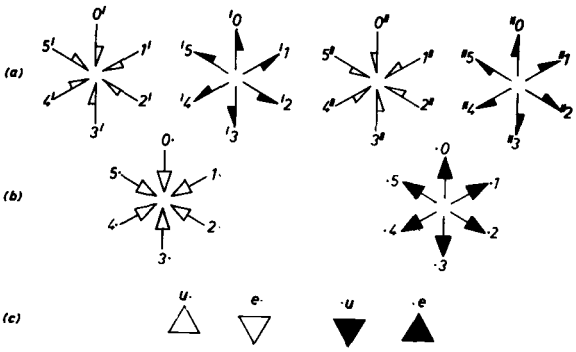

Figure 4. Pictorial representation of packets and their orientational characters. (a) hetero-octahedral; (b) meso-octahedral; (c) homo-octahedral (left = p_{2n}; right = q_{2n+1}).

rotation and are thus of the same enantiomorphous nature. Therefore, in any symbol only one prime or double prime is given between the numbers T_{2n} and T_{2n+1} (similar to the single dot in a symbol for a meso-octahedral mica polytype).

In a *homo-octahedral mica* there are only two possible orientations of any packet p_{2n}; the same holds for packets q_{2n+1}. A displacement of Oc_{2n+1} relative to Tet_{2n} corresponding to the characters 0. or 2. or 4. leads to the same orientation of p_{2n}, a displacement corresponding to characters 1. or 3. or 5., to the other orientation. These orientations are, therefore indicated by the letters e (for even, i.e., 0, 2, 4) and u (for uneven, i.e., 1, 3, 5). The situation is similar for packets q_{2n+1}.

Packet to packet displacements

The displacement of any packet q_{2n+1} relative to p_{2n}, called $v_{2n,\,2n+1}$, is equal to the displacement of Tet_{2n+2} relative to Tet_{2n}. For meso- and hetero-octahedral micas such a displacement is thus equal to the sum of the displacements indicated by the numerical parts of the orientational characters of p_{2n} and q_{2n+1}. As follows from the choice of their origin, the displacement of any packet p_{2n} relative to q_{2n-1} is equal to zero and will be indicated by the character *. In the pictorial representation the shafts of the arrows representing meso- or hetero-octahedral packets are taken of such a length ($a_1/3$) that for a pair pq corresponding to a mica layer their ends coincide.

Full and short polytype symbols

For any *meso-octahedral polytype* the full stacking symbol has the form

$$\begin{matrix} T_0 & \cdot & T_1 & T_2 & \cdot & T_3 & \ldots \\ & v_{0,1} & * & & v_{2,3} & * & \end{matrix} \qquad (3)$$

where any of the characters T_m and $v_{2n,\,2n+1}$ stands for a number 0 to 5. Furthermore, if the vector indicated

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Table 3. Point operations and corresponding conversions of characters.

τ-operation	i	ρ-operation
1	j	1^{-1}
$(6)^{-1}$	1 + j	$(\bar{6})^{-1}$)
$(3)^{-1}$	2 + j	$(\bar{3})^{-1}$
$(2)^1$	3 + j	$(m)^1$
$(3)^1$	4 + j	$(\bar{3})^1$
$(6)^1$	5 + j	$(\bar{3})^1$
′ and ″ remain		′ and ″ interchange
$m \perp b^3$	− j	$2 \parallel b_3$
$m \perp a_2$	1 − j	$2 \parallel a_2$
$m \perp b_1$	2 − j	$2 \parallel b_1$
$m \perp a_3$	3 − j	$2 \parallel a_3$
$m \perp b_2$	4 − j	$2 \parallel b_2$
$m \perp a_1$	5 − j	$2 \parallel a_1$
′ and ″ interchange		′ and ″ remain

by T_m or $v_{2n,\,2n+1}$ is denoted by $\langle T_m \rangle$ or $\langle v_{2n,\,2n+1} \rangle$, respectively, the following relation results:

$$\langle v_{2n,\,2n+1} \rangle = \langle T_{2n} \rangle + \langle T_{2n+1} \rangle. \quad (4)$$

Eq. (4) shows that the second line of symbol (3) follows unequivocally from the first line and is thus redundant. The nonredundant (short) symbol form is

$$T_0.T_1\ T_2.T_3 \ldots . \quad (5)$$

For any given polytype the sequence of numbers and dots in such a short symbol is the same as in the short symbol referring to OD layers introduced above.

For *hetero-octahedral mica polytypes* also, two-line full symbols and one-line short symbols corresponding to symbols (3) and (5) result, with the proviso, that any dot must be replaced by a prime or a double prime (see above). Again the short symbol referred to packets looks exactly like the short symbol referred to layers.

For a *homo-octahedral polytype* the full symbol has also the form of symbol (3), but with $T_{2n} = T_{2n+1}$, where T_{2n} as well as T_{2n+1} may stand now either for e or for u. The first line is redundant as are the asterisks of the second line. The corresponding non-redundant (short) symbol is

$$v_{0,1}\ v_{2,3}\ v_{4,5} \ldots , \quad (6)$$

and the sequence of characters is again the same as that in the symbol (2) referring to layers.

SYMBOLS DENOTING THE SAME POLYTYPE OR ENANTIOMORPHOUS POLYTYPES

The finite sequence of characters between vertical bars stands for an infinite periodic sequence and may be replaced by a finite sequence of the same length starting at a different character of the infinite sequence, without change of the denoted polytype. Symbols differing only in the finite part selected to represent a certain infinite sequence will not be regarded as different.

In addition, rotation of the polytype relative to a chosen triple of basic vectors by a multiple of 60° around an axis parallel to c_0, or by 180° around an axis parallel to a_i or b_i (i = 1, 2, or 3) may change its symbol without changing the polytype. Application of a reflection across a plane perpendicular or parallel to basic vectors leads to the enantiomorph of the original polytype as do the inversion at a point and roto-inversion. The corresponding conversions of characters are governed by the following rules: (1) rotations leave primes and double primes unchanged; (2) any operation leaving a layer or packet upside up i.e., converting a packet p_m into a packet p_n, or q_r into q_s is called a τ-operation and leaves the converted characters in the same sequence as the original characters; (3) any operation turning a layer or packet upside down, i.e., converting a packet p_m into a packet q_n and vice versa is called a ρ-operation and reverses the sequence of converted characters, compared with the sequence of original characters. These relations are indicated in detail in Table 3. Application of a coincidence operation to a polytype corresponds to a conversion of its symbol according to the following rules: Replace any number j of the symbol by a number as indicated in the line marked i; for ρ-operations reverse the sequence of numbers and dots (primes and double primes), for τ-operation keep the sequence; for hetero-octahedral micas keep or interchange primes and double primes as indicated.

Thus, the same polytype is denoted by $|2'0\ 4''0|$ and the following symbols: $|4''0\ 2'0|$ (different start of finite sequence), $|3'1\ 5''1|$ (application of $(6)^{-1}$), $|1'5\ 1''3|$ (application of $(\bar{6})^{-1}$). The polytype $|2.0\ 4.0\ 3.1|$ is enantiomorhpous to $|4.0\ 2.0\ 3.5|$ (applicationof $m|b_3$ and to $|1.3\ 0.4\ 0.2|$ (inversion).

For hetero-octahedral polytypes another ambiguity for the choice of symbols results from the ambiguity in choosing the origin of octahedral layers on the site of any one of the three chemical entities (see Figure 5, central and top part). If a different entity is chosen to fix the origin, the primes and double primes of the symbol remain unchanged, but the numerical parts of characters are changed in a way depending on their position in front or behind a prime or double prime as follows:

$$j' \rightarrow (j + \alpha)' \qquad j'' \rightarrow (j - \alpha)''$$
$$\text{Where } \alpha = 2 \text{ or } -2 \quad (7)$$
$$'j \rightarrow '(j - \alpha) \qquad ''j \rightarrow ''(j + \alpha)$$

As far as the meaning of primes and double primes is concerned, no general rule has been given that states which arrangement of cations in an octahedral layer or packet has to be called right-handed and indicated by a prime. If an arrangement to the previously called left-

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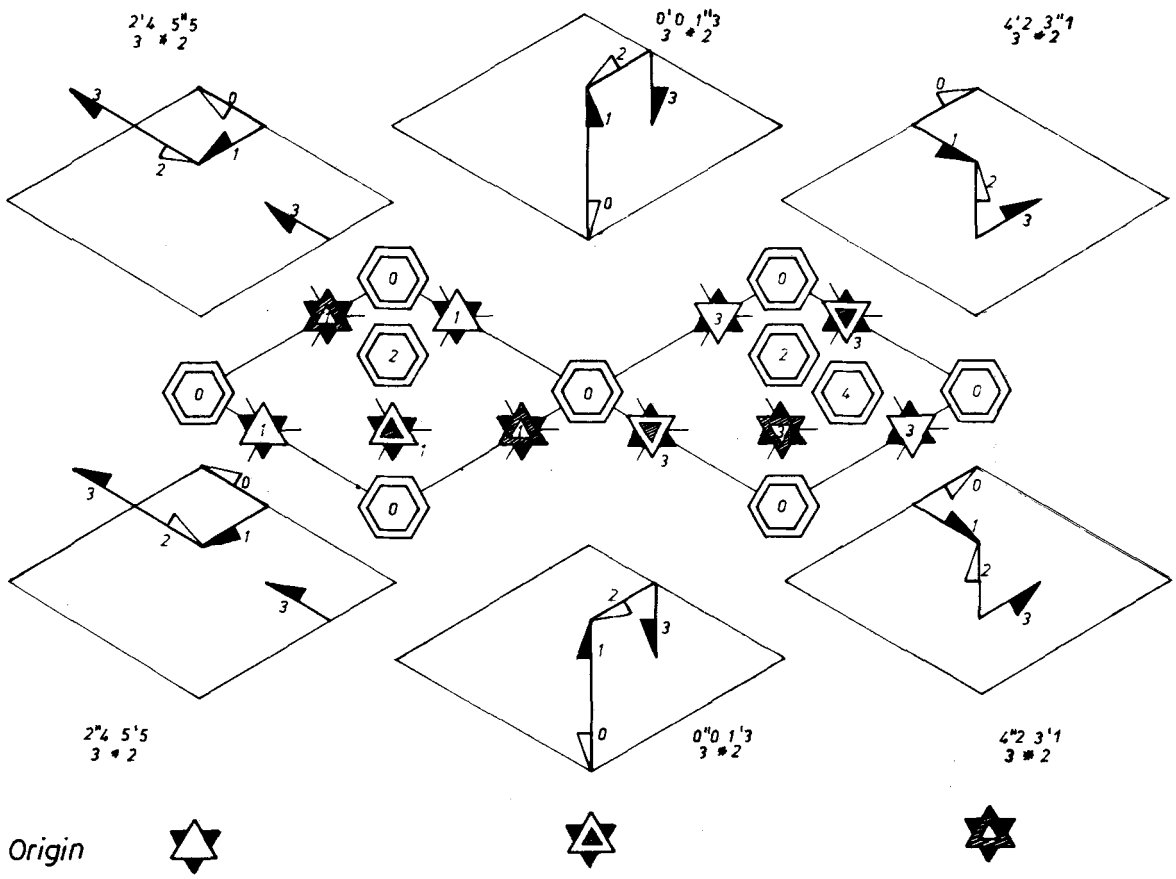

Figure 5. Schematic representation of an arbitrary sequence of five hetero-octahedral layers: (c) by representation of their layers numbered 0 to 4; layers numbered 0, 1, 2 shown in the left unit cell, 2, 3, 4 in the right unit cell; (b) and (d) by representing the four packets contained in the sequence (numbered 0 to 3), referred to the respective origins indicated in (f); (a) and (e) by the symbols corresponding to (b) and (d), respectively.

handed and indicated by a double prime is now called right-handed and indicated by a prime, any polytype is now indicated by a symbol obtained from the original symbol by a replacement of all primes by double primes and vice versa (see the relation between the symbols given in Figure 5a and 5e).

The symbols which, referred to differently chosen origins denote the same polytype (as the symbols given in Figure 5a), obviously denote in general different polytypes, if meant to refer to the same choice of origin. Similarly, two symbols, related to one another by an interchange of primes and double primes (as, e.g., the two symbols of Figure 5a and 5e, both left) denote in general different polytypes, if primes are taken to indicate the same arrangement of chemical entities in octahedral sites. Polytypes denoted by symbols in either of these ways differ, however, only in the occupation of octahedral sites by different chemical entities. They have the same relative position of tetrahedral layers (and thus of silicate sheets). Interchange of primes and double primes of a symbol corresponds to an isomorphous interchange in any octahedral layer of the chemical entities not chosen to fix the origin, i.e., there is an isomorphous replacement of one of these entities by the other and vice versa. Similarly, symbols related as indicated by Eq. (7) denote, if referred to origins fixed in the same way, polytypes related by a cyclic isomorphous interchange of the chemical entities occupying the three octahedral sites (cf. the situation in hetero-octahedral kaolinite-type minerals, Dornberger-Schiff and Ďurovič, 1975b) where these polytypes were called mono-octahedral).

RELATIONS OF HOMOMORPHY BETWEEN POLYTYPES OF DIFFERENT CLASSES

A meso-octahedral polytype has a relation of homomorphy to a homo-octahedral polytype, namely the polytype which would result, if the three octahedral sites of the meso-octahedral mica were occupied by cations of the same kind. The full symbol of the homo-octahedral polytype thus related to a certain meso-octahedral polytype may be obtained from the full symbol

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of the latter by replacing the even or odd orientational characters by the character e and u, respectively, leaving the displacement characters unchanged.

The relation of homomorphy between hetero- and meso-octahedral polytype obtained from the hetero-octahedral polytype by equalizing the different ions not lying on the chosen origin corresponds to the following relations between their full symbols: the symbol of the meso-octahedral polytype is obtained from the symbol of the hetero-octahedral polytype by replacement of primes and double primes by dots. The relation between the symbols of a hetero-octahedral polytype and a homo-octahedral polytype which is obtained from the latter by replacing the three different octahedral cations by cations of the same kind follows from the relations just described: the replacement of even and odd orientational characters of the full symbol of the hetero-octahedral polytype by e and u, respectively, and the primes and double primes by dots.

THE DETERMINATION OF THE SPACE GROUP OF A PERIODIC POLYTYPE FROM ITS SYMBOL

To determine the space group of any periodic mica polytype from its symbol one may proceed as follows:

(1) Determine a translational vector, c' spanning, together with a_1 and a_2, a primitive unit cell.
(2) Take note of any conversion of characters listed in Table 3 which reproduces the sequence of characters in the symbol if applied to its characters one after the other. The corresponding point operations lead to the point group isogonal to the space group.
(3) According to c' (see symbol (1)) and the point group (see symbol (2)), select a triple of basic vectors in keeping with conventions for the crystal class and preferably also to the conventions formulated below, and give the corresponding Bravais lattice.
(4) To any rotations or reflections of the point group find the translational components of the symmetry operations and hence the space group.

With reference to symbol (1), a vector c' is obtained as[5]

$$c' = 2rc_0 + \langle v_{0,\,2r}\rangle, \qquad (8)$$

where 2r is the number of packets per period, and $\langle v_{m,n}\rangle$ (for any of the numbers m, n) denotes the sum $\langle v_{m,m+1}\rangle + \langle v_{m+1,\,m+2}\rangle + \ldots + \langle v_{n-1,\,v_n}\rangle$, indicated by the displacement character $v_{m,\,n}$. Because for any mica polytype $v_{2n-1,\,2n} = *$, it follows that $\langle v_{0,\,2r}\rangle = \langle v_{0,\,1}\rangle + \langle v_{2,\,3}\rangle + \ldots + \langle v_{2r-2,\,2r-1}\rangle$. For meso- and hetero-octahedral mica, 2r is equal to the number of figures between vertical bars of the symbol; for homo-octahedral mica, r is the number of figures between vertical bars of the short symbol.

With reference to symbol (3), for hexagonal, trigonal, and orthorhombic polytypes the displacement vector $\langle v_{0,\,2r}\rangle = 0$, and $c = c'$ and is parallel to c_0. This results from the fact that neither a 3- nor a 6-fold rotation or roto-inversion can occur in any mica polytype. For any hexagonal and trigonal polytype, a_1 and a_2 may be taken as the other two basic vectors. In any orthorhombic polytype there are symmetry planes and/or 2-fold axes referring to a pair of directions parallel to a_i and b_i (with i = 1 or 2 or 3). The vectors a_i and b_i may then be taken as basic vectors a and b, respectively. The Bravais lattice is C. For any monoclinic polytype with symmetry plane and/or 2-fold axis referring to a direction a_i or b_i the vector a_i or b_i, respectively, will be chosen as basic vector b or $-b$ and the other vector as vector a or $-a$; Bravais lattice C. For any monoclinic polytype with symmetry plane and/or 2-fold axis referring to c_0 we way choose $b = c'$. Basic vectors a and c may then either be chosen equal to a_i and a_k, respectively (i, k = 1, 2, 3, $i \neq k$) Bravais lattice P or equal to a_i and b_i, respectively, Bravais lattice C. Generally speaking, $\langle v_{0,\,2r}\rangle$ is in any case parallel to one of the directions $\pm a_i$ or $\pm b_i$, therefore any triclinic polytype may be referred to metrically monoclinic basic vectors with Bravias lattice C.

With reference to symbol (4), in hexagonal and trigonal polytypes the conversions listed under $(6)^{-1}$, $(6)^1$, $(3)^{-1}$, and $(3)^1$ indicate the presence of screw axes 6_5, 6_1, 3_2, and 3_1, respectively. Point operations m $\perp a$ or m $\perp b$ which correspond to a conversion of characters relating any character to itself, indicate mirror planes or b- or a-glide planes, respectively, of the polytype; operations which correspond to a conversion relating different characters indicate c-glide or n-glide planes of the polytype. Symmetry planes perpendicular to c can only be mirror planes connected with n-glide planes. The 2-fold axes parallel to a or to b are necessarily rotation axes connected with screw axes. Any 2-fold axis parallel to c_0 is necessarily a screw axis. From the Bravais lattice, the point group, and by applying the rules given in this paper, the space group then follows.

EXAMPLES

Three examples follow that demonstrate how the space group of a polytype may be deduced from its symbol.

Example 1

Full symbol $\left|\begin{matrix}2.0\ 4.0\\ 1\ *\ 5\ *\end{matrix}\right|$, short symbol $\left|\begin{matrix}2.0\ 4.0\end{matrix}\right|$, quoted by Zvyagin and Soboleva (1974), Zvyagin symbol $s_2s_6t_0s_4s_6t_0$ (see Figure 6).

$$c' = 2c_0 + \langle 1\rangle + \langle 5\rangle = 2c_0 + a_3/3.$$

[5] The vector c_0 is defined as a vector perpendicular to a_1 and a_2, the length of c_0 is defined so that any vector from the origin of the packet p_r to that of p_{r+2} is equal to $c_0 + \alpha a_1 + \beta a_2$ (where α, β depend on the stacking.)

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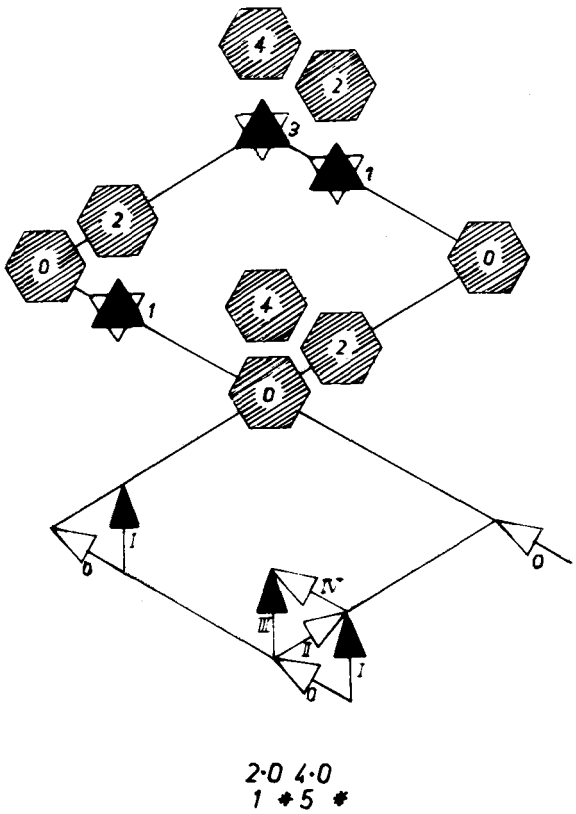

Figure 6. Pictorial representation of the polytype |2.0 4.0|.

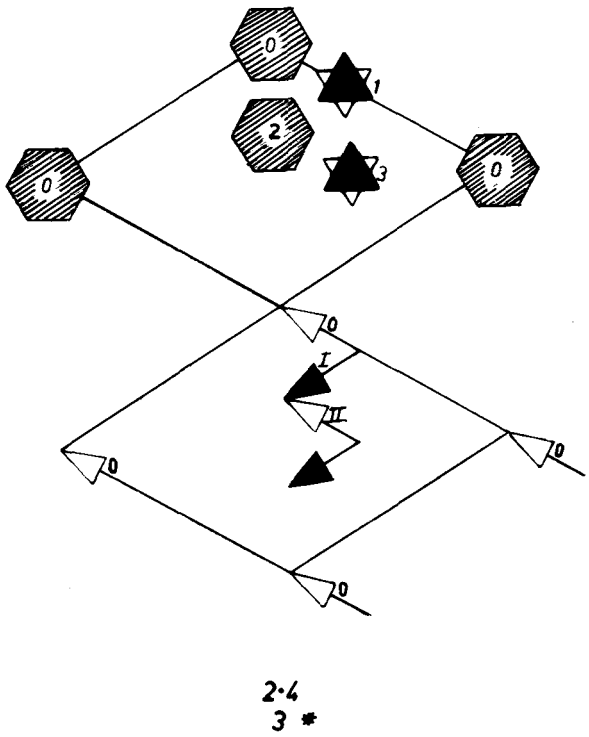

Figure 7. Pictorial representation of the polytype |2.4|.

Rules of conversion: j. into (6 − j). and .j into .(6 − j) hold for characters.

Point operation corresponding to this rule: m ⊥ b_3. Symmetry operation c-glide perpendicular b_3 results. Basic vectors chosen:

$a = -a_3$; $b = -b_3$; $c = 2c_0 - a/3$; Bravais lattice C. Space group Cc.

Example 2

Full symbol $\left|\begin{matrix}2.4\\3\ *\end{matrix}\right|$, short symbol |2.4|, Zvyagin symbol $s_2s_4t_0$ (see Figure 7).

$$c' = c_0 + \langle 3 \rangle = c_0 - a_3/3.$$

Rule of conversion: j. into .(6 − j) and .j into (6 − j). holds for characters with reversal of their sequence.

Point operation corresponding to this rule 2 ∥ b_3. No other relevant rule holds, thus point group 2 follows. Basic vectors chosen $a = a_3$; $b = b_3$; $c = c'$. Bravais lattice C. Space group $C2$.

Example 3

Zinnwaldite, hetero-octahedral, 1M. The following polytype symbols denote 1M polytpyes: |0′0| and |2′4| together with those evidently indicating the same or enantiomorphous polytypes (cf. the first packet pair indicated in Figure 5c, left unit cell, and middle and left part of 5a and 5b). Which of the two symbols is correct depends on the choice of the octahedrally coordinated cation chosen to fix the origin of the octahedral layer.

In either case there is one rule of conversion, namely j′ into ′(6 − j) which corresponds to a 2-fold rotation axis parallel to b. Space group $C2$, with $c' = c = c_0 + \langle 3 \rangle = c_0 - a_3/3$, to be referred to $a = a_3$, $b = b_3$, space group $C2$.

As can easily be seen, the polytype |2.4| (Figure 6) would result from |2′4| (Figure 5(b), left) if the two cations not chosen to indicate the origin were replaced by cations of the same kind (ionic replacement).

The stacking mode of any mica polytype (ordered as well as disordered) can be explained by the stacking of OD layers. By a special procedure, following from OD theory, all possible so-called MDO polytypes (regular or simple polytypes) can be deduced for the given three mica classes. The homomorphic relations between these three classes seem to be useful for the discussion of chemical related micas. For the discussion of real mica structures the ditrigonalization of the tetrahedral sheet must be taken into account. This and an ordered Si/Al substitution are problems to be treated in the future.

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Резюме—С точки зрения симметрии слюды могут быть классифицированы следующим образом: слюды со всеми тремя октаэдрическими координированными местами, занятыми одинаковыми катионами (гомо-октаэдрические слюды), слюды с только двумя местами, занятыми одинаковыми катионами (мезо-октаэдрические слюды), и слюды с тремя местами, занятыми разными катионами либо двумя разными катионами и пустотой в упорядоченной форме (гетеро-октаэдрические сдюды). Для всех этих трех систем, политипы слюд, идеализированные в согласии с обобщенной моделью Паулинга, могут быть интерпретированы как структуры OD, состоящие из октаэдрических слоев OD и тетраэдрических слоев OD, в которых плоскость межслойного катиона замкнута между тетраэдрическими слоями. Слой слюды, построенный из октаэдрического и двух половин тетраэдрических слоев с каждой стороны, состоит из двух пакетов, связанных двойной ротацией.

Ориентация каждого пакета OD может быть описана номером от 0 до 5 (по отношению к гексагональной системе координат). Точка перед либо после этих номеров используется для описания положения октаэдрического слоя (номер + точка = характер ориентации). Перемещение пакета по отношению к его предшественнику характеризуется вектором от начала пакета p_n (или q_{n-1}) до начала соседнего пакета p_{n+1} (или p_{2n}). Эти перемещения могут быть также описаны номерами от 0 до 5 (характеры перемещения); нулевое перемещение означается символом*. Поэтому каждый политип слюды (упорядоченной или неупорядоченной) может быть описан двойным символом. Характеры ориентации расположены в первой линии, а характеры перемещения—во второй. Каждый символ описывает ясно относительное расположение слоев в политипе. Симметрия пространственных групп упорядоченных политипов следует непосредственно из этих символов. [E.C.]

Resümee—Vom Gesichtspunkt der Symmetrie können die Glimmer wie folgt klassifiziert werden: Glimmer, deren 3 oktaedrisch koordinierte Plätze von Kationen gleicher Art besetzt sind (homo-oktaedrisch), Glimmer mit 2 gleichartig besetzten Oktaederplätzen (meso-oktaedrisch) und Glimmer mit 3 verschieden besetzten Oktaederplätzen oder 2 verschieden besetzten plus einer Lücke in geordneter Weise (hetero-oktaedrisch). Für jede dieser 3 Klassen werden die Glimmerpolytypen, entsprechend dem verallgemeinerten Pauling-Modell, als OD-Strukturen aus 2 Arten von OD-Schichten interpretiert, die Oktaederschicht und die Tetraederschicht, die aus der Zwischenschichtkationenebene und den beiden benachbarten tetraedrischen Netzwerken besteht. Eine Glimmerschicht, die aus einer Oktaederschicht und zwei Tetraederhalbschichten aufgebaut ist, besteht aus 2 OD-Paketen, die durch eine zweizählige Achse verknüpft sind.

Die Orientierung jedes OD-Pakets wird durch Ziffern von 0 bis 5 gekennzeichnet (bezogen auf ein hexagonales Koordinaten-system). Ein Punkt hinter oder vor den Ziffern bezeichnet die Lage der Oktaederschicht (Ziffer + Punkt = Orientierungscharakter). Die Verschiebung eines Pakets p_n (oder q_{n-1}) gegenüber dem Paket p_{n+1} (oder p_{2n}) wird durch einen Vektor vom Ursprung des einen zum Ursprung des anderen charakterisiert. Diese Verschiebungen werden ebenfalls durch Ziffern von 0 bis 5 charakterisiert (Verschiebungscharakter). Eine 0-Verschiebung wird durch einen * symbolisiert. Jeder Glimmertyp (geordnet als auch fehlgeordnet) kann nun durch ein zweizeiliges Symbol beschrieben werden. In der ersten Zeile stehen die Orientierungscharaktere, in der zweiten die Verschiebungscharaktere. Jedes Symbol kennzeichnet die Stapelung von Schichten in einem Polytyp eindeutig. Die Raumgruppensymmetrie geordneter Polytypen folgt direkt aus dem Symbol.

Résumé—Du point de vue de la symmétrie, les micas peuvent être classifiés de la manière suivante: ceux dont les trois sites coordonnés octaèdralement sont occupés par le même cation (micas homo-octaèdraux), ceux dont deux de ces sites seulement sont occupés par le même cation (micas méso-octaèdraux), et ceux dont les trois sites sont occupés par des cations différents ou par deux cations différents et par un vide, de manière ordonnée (micas hétéro-octaèdraux). Pour chacune de ces trois classes, des polytypes micas, idéalisés en accord avec le modèle généralisé de Pauling, peuvent être interprétés en tant que structures OD consistant de couches octaèdres OD et de couches tetraèdres OD dans lesquels un plan intercouches de cations est entouré par des feuillets tetraèdres. Une couche mica composée d'un feuillet octaèdre et de deux moitiés de feuillets tetraèdres de chaque côté consiste en deux paquets OD joints par une rotation à double pli.

L'orientation de tout paquet OD peut être donné par un nombre de 0 à 5 (apparenté à un système de coordonnées hexagonales). Un point précédant ou suivant ces nombres est employé pour indiquer la position de la couche octaèdrale (nombre + point = caractère d'orientation). Le déplacement d'un paquet contre son prédécesseur est caracterisé par un vecteur de l'origine d'un paquet p_n (ou q_{n-1}) à l'origine du paquet adjacent $p_{n+1}(p_{2n})$. Ces déplacements peuvent être aussi symbolisés par des nombres de 0 à 5 (caractères de déplacement), un déplacement nul est symbolisé par *. Tout polytype mica (ordonné ou désordonné) peut donc être décrit par un symbole à deux lignes. Les caractères d'orientation sont situés sur la première ligne, et les caractères de déplacement sur la deuxième. Tout symbole, par consequent, indique de manière unique l'assemblage de couches d'un polytype. La symmétrie espace-groupe de polytypes ordonnés suit directement du symbole.[D.J.]

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