CURRENT PROBLEMS WITH THE NOMENCLATURE OF PHYLLOSILICATES*

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Abstract—The nomenclature of phyllosilicates is discussed in relation to structural variations of layers and interlayers. Some discrepancies in the nomenclature which arose due to historical reasons and different viewpoints may be reconciled if the choice of the construction units (layers or their parts) is related to definite sets of structures for which these units are common. Features of idealized models approximating real structures should be considered for classification and derivation of nomenclature sets, whereas priority is given to structural variations before lattice and symmetry characteristics. Layer polymorphs, pseudo-polytypes, polytypes (both simple and complex), and OD structures are distinguished. Particular results obtained for micas as a model example of phyllosilicates in relation to modular structures in general are considered in an Appendix.

Key Words-Construction Unit, Nomenclature, Phyllosilicates.

INTRODUCTION

The nomenclature of phyllosilicates has been considered many times and has evolved over time (*e.g.* Bailey, 1980; Guggenheim, 2000). Attention is paid here to some current problems relating to structural variations of phyllosilicates and data from electron diffraction studies.

Electron diffraction, as an independent source of structural information, requires evaluation and generalization of results featuring the investigated objects. In particular, electron diffraction texture patterns are especially effective for layer structures because they display separately the features of the layers and how the layers are stacked. Therefore, electron diffraction applications have produced refinements or even a revision of results obtained from other techniques, which have led to changes in ideas and conclusions, such as in areas of polymorphism, polytypism and order-disorder (OD) diversity. These areas are of special interest when applied to phyllosilicates and clay minerals, in particular.

The nomenclature problems under consideration are closely related to the modular aspects of minerals. The general relationships between modular crystal structures and specific results obtained for mica phyllosilicates illustrating the ideas presented here are given in the Appendix.

STRUCTURAL UNITS AND NOMENCLATURE

The AIPEA Nomenclature Committee (Brindley and Pedro, 1972) distinguished single atomic planes, sheets, layers, interlayers and their combination into unit structures, which define different phyllosilicates independently of their chemical features. Thus, kaolin minerals and serpentines are distinguished by OT or 1:1 layers where O = octahedral and T = tetrahedralsheets, dioctahedral (di) and trioctahedral(tri) micas by TOT + X or 2:1 layers separated by X interlayer atomic planes, pyrophyllite and talc by TOT or 2:1 layers and vacant interlayers, and chlorites by unit structures TOT + O or 2:1 + 0:1 where O sheets may be both trioctahedral and dioctahedral forming unit structures tri-tri, di-tri or di-di. These combinations of layers, sheets and planes may be referred to as nomenclature units.

Two nomenclature committees (Bailey, 1977; Guinier, 1984) were commissioned to define the notion and symbols of polytypes. However, these committee reports were not complete and allowed different interpretations, ranging from those given by Dornberger-Schiff and Durovic (1975) and Dornberger-Schiff (1982), to those of Angel (1986). Structures, based on definitions given to polytypes, "may be regarded as built up by stacking layers . . . and differ in their stacking sequence" (Guinier, 1984). However, these structures may have specific general features that are not common to all of them but are distinctive of certain groups. These differences in general features cannot be neglected and should affect the nomenclature.

Thus, the same atomic planes may compose different sheets (*e.g.* octahedral (O) sheets or prismatic (P) sheets) where the outer anionic planes occupy equivalent positions defined by the symmetry of the intermediate cationic plane. Sheets may form layers having coincidently non-equivalent structures. Tetrahedral and dioctahedral sheets may form TOT layers with *trans*or *cis*-vacant octahedra. If the relative orientation (same or opposite) of the basal faces of adjacent sheets

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T and O is fixed, then the T sheets of the trans-vacant and cis-vacant TOT layers are related within the O sheet by centers of symmetry together with two-fold axes or only by two-fold axes, and the TOT layers have ideal symmetries C2/m and C2, respectively. These layers may be designated CS (centrosymmetric) and AS (axially symmetric), respectively. Furthermore, tetrahedral rotation, the in-plane rotation of tetrahedra around the normals to the basal plane passing through the tetrahedral centers, may provide 2:1 layers differing in relative orientations of adjacent O and T sheets. According to approximate cubic (c) or hexagonal (h) close packing positions of two inner (O, OH) planes, the TOT layers may be described as cc, hh or ch (hc). Franzini (1969) distinguished two kinds of mica layers, A and B, which correspond to TOT layers cccc and chhc. The positions c of the outer O planes of these layers define a layer stacking, which provides octahedral coordination for the interlayer cations both with the same or alternating parities of layer orientations, as in micas $2M_1$ and $2M_2$, respectively. Actually, instead of layers B, layers cc were found, at least for dioctahedral micas $2M_2$ (Zhukhlistov et al., 1973) where the outer O planes of adjacent TOT layers are directly superimposed and violate the close packing. Layers with outer planes in positions h may form pyrophyllite polytype structures and are characteristic of semiconductor sulfides also composed of TOT layers and vacant interlayers (Zvyagin and Kyazumov, 1993).

There are various possibilities for the choice of twodimensional units in phyllosilicate structures that are useful in different respects (description, display of the lattice, the symmetry, and the diffraction features (Zvyagin, 1967; Takeda and Sadanaga, 1969; Dornberger-Schiff and Durovic, 1975)). Operation with some parts of the nomenclature units defining the phyllosilicate types (e.g. with non-polar O sheets and polar T sheets) present the structures of phyllosilicates as polytypes (Zvyagin, 1967). However, essential differences in some of them expressed by the nomenclature units are then lost. Therefore, the notion of polytypism in phyllosilicates is to be related to the nomenclature units that define the status of kaolins, micas, etc. Those polytypes, which differ by the fixed structure of these units, belong to different polymorphs of the corresponding phyllosilicate. This is the case with 2:1 TOT trans- and cis-vacant or CS and AS layers (see the Appendix). Such polymorphs were identified by means of electron diffraction for micas, illites and smectites (Tsipurski and Drits, 1984; Zvyagin et al., 1985; Zhukhlistov and Zvyagin, 1991), and, in principle are possible for pyrophyllite and dioctahedral chlorite. The status of different polymorphs also may be attributed to micas differing in relative orientations

of their T and O sheets like the micas built of A and B layers considered by Franzini (1969). Apart from pure polymorphs, mixed-polymorphs can form the alternation of layers differing in their fixed structure. On the other hand, with the use of, *e.g.* single T and O sheets or of TOT-layer halves (Zvyagin, 1967; Zvyagin *et al.*, 1979) as units constituting polytype structures, the polymorph features above are lost.

With the choice of constructing layers fixed, the stacking in a phyllosilicate structure may form different interlayers, and one must distinguish such structures based on this feature. Each kind of interlayer defines a group of polytypes because nearly identical layers and similar interlayers are a general feature of polytype structures. The phyllosilicates, which differ in their interlayers, may be considered as pseudo-polytypes intermediate between pure polytypes and polymorphs. This is the case with micas where successive layers have the same (S) or alternating (A) parity of azimuthal orientations (related by rotations through either even or odd numbers of 60°, respectively). At the ditrigonal geometry of T sheets and their fixed orientation relative to the adjacent O sheet, the interlayers S and A differ in the octahedral ('O') or prismatic ('P') coordination of the interlayer cations, respectively. The interlayers may then be designated as O or P interlayers, respectively (Appendix). The prismatic coordination of the interlayer cations was confirmed in an electron diffraction study of muscovite $2M_2$ (Zhukhlistov et al., 1973). Different interlayer configurations may be combined in a sequence of layers with some non-alternating mixed-parities (M) of layer orientations to form a mixed-interlayer (O, P) pseudopolytype.

Polytypes may be simple or complex. In simple polytypes, the successive layers are related by transition operations that produce equivalent results. In complex polytypes, operations characteristic of different simple polytypes are combined. The status of simple and complex is dependent on the diversity of operations involved and on the choice of the layer units forming the structure of the polytypes. Thus, reflection operations must be considered for AS (cis-vacant) 2:1 mica layers, in addition to translations and rotations as recommended by Bailey (1977) and Guinier (1984). With the use of the condition of equivalent transitions between successive 2:1 layers (homogeneity condition), 18 simple polytypes of CS and AS micas instead of the 6 for CS micas were derived, and these are distributed systematically over the mica polymorphs and pseudo-polytypes (Zvyagin and Zhukhlistov, 1999; Appendix, Tables 1 and 2). Operation with the "OD-packets" of Backhaus and Durovic (1984), which are equivalent to polar (TOT+X)/2 units, produced 14 simple polytypes of meso-micas analogous

to dioctahedral micas. The OD approach ignores the features of polymorphs and pseudo-polytypes consisting of 2:1 mica layers.

A complex problem in the nomenclature of phyllosilicates is the relationship between polytypes and OD structures. The term OD (order-disorder) implies that pairs of adjacent layers are symmetrically equivalent for some set of layer structures (Dornberger-Schiff, 1964). However, the phenomenon of polytypism itself does not require such a condition and no restrictions exist for the layers. The structure of the layers should be fixed and several equivalent variants of their stacking provide the diversity of layer structures (polytypes). However, it is just the freedom of choice of constituent layers that was the reason for considering polytypism and OD as synonyms (Dornberger-Schiff, 1982). The OD interpretations were given to phyllosilicate structures with another choice of the so-called building layers (BL), which are certain parts and even atomic planes of the nomenclature units, which were accompanied with increasing numbers of layer types (Dornberger-Schiff and Durovic, 1975; Durovic, 1981; Dornberger-Schiff et al., 1982). Depending on the success in finding OD layers, which are, to some extent, artificial and not always obvious, such an interpretation complicates the understanding of polytype nomenclature. For phyllosilicates, use of single atomic planes as original constructive units is not justified, because atomic interactions inside a plane and between adjacent planes are of the same order of magnitude and the arrangement of these planes may not be subjected to differences in stacking.

On the other hand, these OD interpretations obscure the real OD structures that exist among both simple and complex polytypes. For example, according to the electron diffraction data for halloysite (Chukhrov and Zvyagin, 1966) the pairs of 1:1 layers of kaolinite and halloysite are symmetrically equivalent (related by a reflection operation). These polytypes can be considered as real OD structures. In contrast, pairs of 1:1 layers in kaolinite and dickite polytypes are independent (cannot be transferred from one to another by any symmetry operation) and do not form OD structures. This difference in these examples must not be overlooked, as it happens within an OD interpretation with the special choice of layers and increased numbers of layer types (Dornberger-Schiff and Durovic, 1975).

FEATURES RESPONSIBLE FOR INCORPORATION OF PHYLLOSILICATES INTO NOMENCLATURE SETS

Any nomenclature set of crystal structures is defined by some general features, which are common for all its members. In the case of polytypes and OD structures, these features are the construction of layers and rules for their stacking. However, layers and interlayers are, in fact, not strictly identical for members of a set just because of differences in their layer-stacking order. These are layers and interlayers of ideal models approximating the real structures, which are common to all the members of a nomenclature set and define its originality. Ideal models are useful for preliminary considerations and operations, and they can serve for theoretical derivation-prediction of layer structures composing a nomenclature set. The terms dioctahedral and trioctahedral, trans-vacant (CS) and cis-vacant (AS) concern ideal layer models that can form various structures as a result of stacking variations, although in real structures, the ideal layer symmetry may be distorted and layers may not be strictly identical in different polytypes. The real kaolinite 1:1 layers, for example, cannot form the dickite structure and vice versa (Zvyagin and Drits, 1996). Likewise, the homo-, meso- and hetero-distributions of octahedral cations (Dornberger-Schiff et al., 1982) are not always known characteristics of a particular (real) mica structure. The actual distribution of isomorphous substitutions of octahedral cations is not a cause of but rather a result of stacking order differences for particular polytype structures. Such features of real structures may be profitable for the realization of a single polytype but not for the others permitted by ideal models. They may not be retained in the latter or even prevent the latter from their formation, and they cannot be used in the theoretical derivation of polytypes.

AXIAL SETTINGS, LATTICE FEATURES AND SYSTEMATICS OF PHYLLOSILICATES

Layer structures pertaining to a nomenclature set require coordinate systems with a common unit-cell basis (ab) defined by the lateral dimensions of all layers. Then, the lattice features of the set members are reduced to the number N of layers per repeat and the normal projection c_n , of the axis c on the (001) plane. Phyllosilicates are described on an ortho-hexagonal basis with $b = a\sqrt{3}$. The normal projections c_n are vector sums of successive intersheet displacements s_i (see the Appendix, Figure 1) per layer repeat and may be reduced to three kinds: [0, 0], $[-\frac{1}{3}, 0]$, and $[0, -\frac{1}{3}]$. These define unit-cells, one of which is orthogonal and two are monoclinic with an obtuse angle either β or α independent of the real symmetry (monoclinic or triclinic) of the structures (Zvyagin, 1967). These unitcells do not correspond to the axial settings designated as 20, 1M and $2M_2$ for micas (Takeda and Sadanaga, 1969). The specific choice (one of six) of the axes aand b depends on the symmetry of the structure formed by the sequence of layers. Given the designations of these axes (a and b), it is reasonable not to interchange for structures of a polytype set with different monoclinic faces of the unit-cell. The tilts of the axes c to the ab plane depend on the number N of layers per repeat.

The uniqueness of polytype and OD structures is defined completely by their fixed units, rules for unit stacking, and stacking sequences of the units. In general, the structural units may comprise any infinite or finite parts of a crystal structure (layers, rods, blocks). However, layers are accepted as model units because they display the most important and widespread case, and with their use all general principles of description, analysis of periodicity, symmetry, and equivalence-independence relationships for members of a set may be better formulated.

In contrast to the structure of layers and interlayers, which serve as general features distinguishing nomenclature sets, symmetry and lattice are characteristics of a particular layer structure. Similar *N* values and kinds of unit-cell shapes may occur among different phyllosilicates. Even for a single type of phyllosilicate, these features do not express directly an additional relationship of crystal-chemical importance. Of course, one can calculate the number of polytypes corresponding to some number of layers per repeat or to some unitcell shape, but this is of theoretical interest. Therefore these features are not suitable for classification purposes. An attempt to use them in such a respect may lead to confusion.

Thus, according to the nomenclature described, *e.g.* by Nespolo (1999), the CS-mica pseudopolytypes A-2 M_2 (I-symbol 45, Appendix) and S-3 TC_1 (446) (Ross *et al.*, 1966) of subfamilies B and A differing in interlayers ('P' and 'O', respectively) belong to a common lattice class b. In contrast, true mica polytypes $3TC_1$ and $2M_1$ (24) (same interlayers 'O') of the subfamily A should fall into different lattice classes, b and a. The lattice classes are uniting pseudopolytypes and separating true polytypes. Thus, the natural relationships between the phyllosilicates are disturbed.

It is instructive to compare the subdivisions of the 26 four-layer mica structures derived by Takeda and Ross (1995) according to their lattice (c_n values) and structural (S, A, M) features:

$$26 = 6([0, 0]) + 14([-1/3, 0]) + 6([0, -1/3])$$

= 4S + 5A + 17M;
$$4S = 4([-1/3, 0]),$$

$$5A = 3([0, 0]) + 2([0, -1/3]),$$

$$7M = 3([0, 0]) + 10([-1/3, 0]) + 4([0, -1/3]).$$

All four-layer mica polytypes are complex. Two of them, one of type S ($4M_3$, I-symbol 1353) and one of type A ($4M_6$, 2343), belong to OD families including simple mica polytypes $2M_1$ and $2M_2$, respectively. Micas *M* (*e.g.* $4M_5$, 2346) cannot belong to an OD family

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since layers in pairs have relative rotations that are multiples both of 120° and of 60° . Within the same lattice, the polytypes differ in their symmetry (rhombic, monoclinic, triclinic); within the same symmetry, they differ in the specific space groups, and within the same space group they differ in the arrangement of symmetry elements inside the structure (*e.g.* with respect to layers and interlayers). It is evident that S, A and M features unite these structures into nomenclature sets whereas the lattice and symmetry features are specific for particular polytypes belonging to the S, A or M type.

CONCLUSIONS

Nomenclature problems are always a matter of discussion and often a source of disagreement. The considerations above about specifying constructive units, operation with ideal models that approximate real structures, and the priority of structural features above lattice features may clarify the situation.

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APPENDIX



Figure 1. Six choices for the layer axes a_i (i = 1, 2, ..., 6) and six intralayer intersheet displacements s_i resulting from the vector a/3 by layer rotations bringing the axis a_i in coincidence with the structure reference axis a. The coordinate axes and displacement vectors are imaged on the background of the upper octahedral bases (thin lines) combined with the projection of the hexagon of T cations (bold circles) under the situation when a_3 is parallel to a. The same sextuple of vectors having absolute values a/3 also represent the stagger vectors $v_i = s$, at l = i.

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315	642	33 11 55	$\widehat{\mathbf{S}}$	51 35 13	(2)	15 53 31	(4)	51 53 13 15 35 31	(17)	15 35 31 51 53 13	(17)
54	21	55 44	14	13 62	20	31 26 ((20)	13 26	16	31 62	(16)
36	63	33 66	×	51 24	6	15 42	6	51 42	13	15 24	13
15,612	612,345	33 44 55 66 11 22	10	51 62 13 24 35 46	11	15 26 31 42 53 64	12	51 26 13 42 35 64	18	15 62 31 24 53 46	18
!1,654	654,321	33 22 11 66 55 44	(10)	51 46 35 24 13 62	(12)	15 64 53 42 31 26 ((11)	51 64 35 42 13 26	(18)	15 46 53 24 31 62	(18)
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Table 1. Mica structures with a regular alternation of layer orientations and simple polytypes.

Clays and Clay Minerals

No.	ii	ij, ji	ij/ji; ji/ij	ii, ij	ij/ji
S1	C2/m	C2	C2/c	1 <i>M</i>	$2M_1$
S2	C2/c	C2	Cc	$2M_1$	$2M_1$
S3	$P3_{1}12$	$P3_{1}12$	P3,12	$3T^{-}$	6T
S4	P3,12	$P3_{2}12$	$P3_{1}12$	3 <i>T</i>	6T
A1	$\tilde{C2/c}$	$C2^{}$	$Cc^{}$	$2M_2$	$2M_2$
A2	Ccmm	$C222_{1}$	Cc2m	20^{-}	20
A3	$P6_{1}22$	$P6_{1}22$	P3112	6H	6T
A4	P6 ₅ 22	P6522	$P3_{2}12$	6 <i>H</i>	6T

Table 3. Characters.

Z	DBD	
3	0	
4	5	
5	4	
6	3	
1	2	
2	1	

Characters, 'Z-', according to Zvyagin (1964, 1967, 1988) used here, 'DBD-', according to Dornberger-Schiff et al. (1982).

Table 4. Symbol relationships.

				5 ¹
Ι	L = l	ii	ij	ji
3	6	33	51	15
4	1	44	62	26
5	2	55	13	31
6	3	66	24	42
1	4	11	35	53
2	5	22	46	64

EXPLANATORY NOTES

The systematics scheme displays the relationships between different modular structures according to a sequence of features ranging from more general to more specific. The general principle of its construction is the same as used by Angel (1986). He considered only three levels and distinguished different kinds of modular structures as polytypes I, II, IIIa and IIIb. The purpose of a more detailed scheme (Zvyagin, 1993) was to display the meaning of notions that are used widely for different forms of modular structures and to reveal the relationships between them. The present scheme is a refinement of the previous one (Zvyagin, 1993) where examples are also given of modular structures corresponding to the features indicated. The term module is related not to a single structure but to some set of structures for which this module is common, and the module choice is defined by this set. Thus, T and O sheets are common to all phyllosilicates. Certain combinations of these sheets are featured in more restricted sets of phyllosilicates. OT layers, TOT layers bordered by interlayer halves are modules found only in kaolins (serpentines), illites (micas), smectites and pyrophyllites (talcs). Dioctahedral TOT layers, CS and AS, provide a further subdivision of the corresponding phyllosilicates into further restricted sets. Depending on their stacking, these modules form different kinds of single-module structures in the left branch of the scheme. Their interstratification within individual crystals forms mixed-layer structures, e.g. illite-

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smectites, placed in the right branch of the scheme. Chlorites are composed of two kinds of modules, O and TOT, which if taken separately, can be attributed to brucite-gibbsite (B) and talc-mica (M), respectively. The regular alternation of B and M (BM) satisfy the featured conditions for polysomes and hybrids. Depending on the stacking, they may form polytypes and OD structures. The notion of polysomes also comprises structures differing in relative amounts (and hence in chemical composition) and alternation order of their modules (Thompson, 1978). This is the case with the pyroxene-spinel (P-S) polysomatic system (P and S modules are layer slices cut normal to the close-packed planes of oxygen atoms). The regular alternation PS in sapphirine polytypes and OD structures represent one member of the set P_mS_n ranging between P and S end-members (Merlino and Zvyagin, in prep.).

With regular alternation PS, the symmetry of the S modules provides two equivalent variants for triples PSP. One is characteristic of sapphirine polytypes and OD structures where the Si tetrahedra form branched chains. The other provides a set of polytypes and OD structures where the Si tetrahedra are grouped into sheets combined with isolated tetrahedra. Both sets represent two polymorphs and, hence, two polytype families united in one and the same OD family, since layer pairs PS (SP) are symmetrically equivalent for all the structures.

Modules may be considered as original if they are present only in combination with substantial modules. Thus, carlosturonites (Compagnoni *et al.*, 1985) are composed of serpentine slices [$S = M_2T_2O_5(OH)_4$]_m alternating with singular slices $X = M_6T_2O_3(OH)_{14}$. The latter, taken separately, do not form any known crystal structures and are examples of original modules. The characteristic features present a sequence of general notions designating some particular cases of modular structures: Modular Structures—Polysomes—Mixed-layer Structures—Hybrids—Polytypes—OD-Structures. It is not a completely hierarchical sequence. Thus, each polytype group includes members, some of which are and others of which are not OD structures. However, as indicated above, there are also groups of OD structures which unite different polytype groups belonging to different polymorphs. Different polymorphs and pseudopolytypes may be formed from layer-modules of one kind and are of particular importance in the nomenclature of micas (see the corresponding scheme).

The letters in the mica nomenclature scheme mean: X interlayer cations; T—tetrahedral sheet; O—octahedral sheet or interlayer; P—prismatic interlayer; S, A, M—same, alternating and mixed parities of layer orientations; OD—orderdisorder; MDO—maximum degree of order.

Characters *i*, *j* belong to a circular succession 1, 2, ..., 6 and are indices of intralayer intersheet displacements \mathbf{s}_{p} \mathbf{s}_{j} characterized by their normal projections on the plane *ab* in the coordinate system of the sequence of TOT layers (Figure 1). These displacement vectors are relating the upward succeeding sheets TO and OT in a TOT layer respectively. The origins of the T sheets are in the centers of the hexagons of T cations, the origins of the O sheets are in the centers of vacant octahedra of dioctahedral TOT layers and in octahedra centers which are symmetry centers of trioctahedral TOT layers. Symbols (index pairs) *ii* characterize CS TOT layers (both di- and tri-), symbols *ij* ($i \neq j$) designate AS dioctahedral TOT layers.

The orientations of layers TOT are defined by their stagger \mathbf{v}_l = $\mathbf{s}_i + \mathbf{s}_j$ and described with characters L = l, or $I = l \pm 3$, since for CS layers *ii* $\mathbf{v}_l = 2\mathbf{s}_i$ which for ideal models (s = a/3)

Nomenclature systematics of the micas

Feature Nomenclature Layers (X/2)TOT(X/2) micas Intralayer intersheet ii ij (i≠j) ii, ij polymorphs displacements and mixed $s_i s_j$ O'.'P' polymorphs (M) ٥' ΎP Interlayers 'O', 'P °O' ۰p 'O', 'P °O' ٩[,] pseudopolytypes (Orientation parities) (S) (A) (M) (S) (A) (M) (S) (A) Stacking simple complex simple complex simple complex simple complex polytypes sequences OD OD Laver OD OD OD OD OD OD **OD**-structures (MDO)pairs (MDO)(MDO) (MDO)

equivalence

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are translationally equivalent to $s_{i\pm 3}$. The values $I = L \pm 3$ define the particular layer axis a_i which is parallel to the reference axis a of the whole structure according to Figure 1.

The mica structures are described with successive orientational characters I and L and index pairs *ii* or *ij* corresponding to a layer succession per layer repeat. According to the symbol transformations accompanying different symmetry operations (Zvyagin *et al.*, 1979; Zvyagin, 1997) such notations express the main general structural features: equivalence-independence, periodicity, space symmetry and distribution of symmetry elements over layers and interlayers, equivalence relationships of layer pairs and other groups of successive layers featuring OD structures, simple and complex polytypes.





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