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Representation of the Axial Settings of Mica Polytypes

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Abstract

The basic unit of mica polytypes has monoclinic symmetry and the layer stagger is a submultiple of the periodicity along the a axis. Because of these features, more than one suitable axial setting can be chosen for non-orthogonal micas. Three types of axial settings are introduced and shown to be useful for classifying non-orthogonal polytypes of micas and indexing their diffraction patterns. *Standard setting* is the axial setting of a polytype leading to the shortest projection of the c axis onto the (001) plane. *Basic axial setting* is the standard setting of a polytype with a number N of layers equal to an integral multiple of 3^n. All the polytypes having the same basic axial setting belong to the same *Series*. *Fixed-angle setting* is the axial setting of a general polytype showing the same angle as the corresponding basic axial setting. The total layer stagger of stacking classifies polytypes into two *Classes*: their c axis is inclined towards respectively the shortest (*Class a*) or the longest (*Class b*) of the two orthohexagonal axes in the plane of the layer. Each *Class* is further divided according to $N = 1\,(\mathrm{mod}\,3)$ (*Subclass*1) and $N = 2\,(\mathrm{mod}\,3)$ (*Subclass* 2). By expressing N as $3^n(3K + L)$, the two integers n and L (1 or 2) establish the *Series* and the *Subclass*, respectively. This definition allows an effective classification of the polytypes and a systematic approach to the indexing of diffraction patterns, independently of their complexity, which increases with N. The transformation rules between settings are given and examples are discussed.

1. Introduction

Approaches using numeric representations (Ross *et al.*, 1966; Takeda & Sadanaga, 1969; Zvyagin, 1962, 1967, 1974; Zvyagin *et al.*, 1979; Dornberger-Schiff, Backhaus & Ďurovič, 1982; Dornberger-Schiff, Ďurovič & Zvyagin, 1982; Backhaus & Ďurovič, 1984; Ďurovič *et al.*, 1984; Weiss & Wiewióra, 1986; Zhukhlistov *et al.*, 1990; Takeda & Ross, 1995), vector schemes (Smith & Yoder, 1956; Takéuchi & Haga, 1971) or both (Dekeyser & Amelinckx, 1953; Thompson, 1981) have been introduced to describe mica polytypes, whose features derive from the stacking in a complex way of a simple unit layer (Hendricks & Jefferson, 1939). Mica polytypes exhibit local symmetry higher than that shown by their space group and unit-cell translations (Sadanaga & Takeda, 1968).

The choice of the axial setting represents an important step in comparing calculated and experimental patterns, especially when the number of layers increases. Different axial settings have been used in the literature; in some cases, the projection of the c axis onto the (001) plane was kept constant, in others, it was the monoclinic angle, and in others neither was kept. Furthermore, examples can be traced where a mix of different axial settings is used to index different reciprocal-lattice planes of the same polytype or where the setting of a polytype is used to index the pattern of a different polytype (Ross *et al.*, 1966; polytypes $3T$, $3A_1$, $4M_1$, $4M_2$, $4M_3$, $4A_8$).† In the present work, the axial settings for mica polytypes are for the first time defined in a systematic way and the transformation rules between them are given. This is the first treatment leading to a completely general approach to the problem of the choice of mica axial settings. It might also be used as the starting point for similar generalizations in cases of other phyllosilicates, which share many geometrical features with micas.

In the following, we shall constantly refer to the space-fixed orthohexagonal reference introduced by Zvyagin (1962). However, different structure-related axial settings will be introduced in both direct and reciprocal space. The relation with Zvyagin's setting will be kept by means of the transformation matrices, which will be given according to Hahn (1983) and Arnold (1983): covariant and contravariant quantities written as row and column matrices, respectively. According to Hahn (1983), bold letters (*e.g.* **a**, **b**, **c**) indicate vectors, while their lengths are written as standard italic letters (*e.g.* a, b, c); axes are also written as standard italic letters.

† According to the suggestions of the IUCr *Ad Hoc* Committee on the Nomenclature of Polytypes (Guinier *et al.*, 1984), the lattice symbol for triclinic polytypes should be changed from Tc to A (anorthic). The polytype called $4A_1$ in Ross *et al.* (1966) has been called $4A_8$ in Takeda & Ross (1995) and *vice versa*.

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Table 1. *Metrical relations in orthohexagonal and monoclinic settings*

Orthohexagonal setting			Monoclinic setting		
$b = a \times 3^{1/2}$	$\left\{\begin{array}{c} a^* = 1/a \\ b^* = 1/b \\ c^* = 1/c \end{array}\right\}$	$b^* = a^*/3^{1/2}$	$b = a \times 3^{1/2}$	$\left\{\begin{array}{c} \beta^* = \pi - \beta \Rightarrow \sin\beta = \sin\beta^* \\ a^* = 1/a\sin\beta^* \\ b^* = 1/b \\ c^* = 1/c\sin\beta^* \end{array}\right\}$	$b^* = a^* \sin\beta^*/3^{1/2}$

2. Unit layer

The ideal mica unit layer is built up by sandwiching an octahedral (O) sheet with symmetry $P(\bar{3})1m$ [notation after Dornberger-Schiff (1959); details in Merlino (1990)] between two tetrahedral (T) sheets with symmetry $P(6)mm$, which is reduced to $P(3)1m$ by the so-called ditrigonal rotation within the tetrahedral sheet (Radoslovich, 1959; Radoslovich & Norrish, 1962; Takeda & Sadanaga, 1969). The two T sheets show a relative shift of $a/3$ so that the resulting layer symmetry is finally $C12/m(1)$ (Pabst, 1955). Rare cases of non-centrosymmetric layers (*e.g.* Brown, 1978) are neglected in this paper. The symmetry of the single layer structure ($1M$ polytype) is $C2/m$, b-unique setting. Two adjacent T sheets belonging to different layers are always exactly facing each other in the ideal structure [$P(6)mm$ symmetry of the tetrahedral sheets].

Neglecting small deviations from ideality, all mica polytypes are based on a hexagonal plane lattice [(001) plane], while in three dimensions they are metrically at least monoclinic.† The ideal mica lattice can thus be monoclinic, orthorhombic or trigonal and hexagonal: in the plane of the layer, two hexagonal axes a_1 and a_2 can be chosen but the axial setting based on them is useful only in dealing with trigonal and hexagonal polytypes. A C-centred unit cell, based on orthohexagonal a and b axes (orthohexagonal metric: $b = a \times 3^{1/2}$, $\gamma = \pi/2$) and with the shortest c axis, displays the complete symmetry of the layer. This is the cell most commonly used to describe the $1M$ polytype and it is called the conventional cell according to Burzlaff *et al.* (1983). The reduction algorithm to the reduced cell is well known. Here the orthohexagonal a and b axes, corresponding to the cell called C_1 in Arnold (1983), is adopted. Finally, for all mica polytypes, a multiple (ideally) orthohexagonal cell can always be chosen whose axes will be kept coincident with those of Zvyagin's space-fixed reference. For non-orthogonal N-layer polytypes, it can be obtained by stacking three N-layer repeats. The metrical relations in direct and reciprocal space, in both the orthohexagonal and monoclinic settings, are given in Table 1. If c' is the vertical axis of the orthohexagonal sextuple cell and c that of the monoclinic cell, keeping unchanged the orientation of the axes in the plane of the layer, the transformation between monoclinic and orthogonal C_1 setting is as follows:

$$
\begin{aligned}
&(a \quad b \quad c')\Pi = (a \quad b \quad c), \\
&\Pi = \begin{bmatrix} 1 & 0 & \frac{\bar{1}}{3} \\ 0 & 1 & 0 \\ 0 & 0 & \frac{1}{3} \end{bmatrix}, \quad V = V'/3, \\
&(a \quad b \quad c)\Pi^{-1} = (a \quad b \quad c'), \\
&\Pi^{-1} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{bmatrix}, \quad V' = 3V.
\end{aligned}
\qquad (1)
$$

3. Classification of polytypes

An N-layer mica polytype is built by stacking N layers with a rotation between successive layers that is an integral multiple of 60° (Smith & Yoder, 1956). Geometrical features of mica polytypes can be simply expressed with the aid of two parameters (notation from Zvyagin, 1997): $\mathbf{c}_n$, which is the projection of the c axis on (001), and $\mathbf{c}_o$, which is the projection of the c axis on the c^* axis. The projection $\mathbf{c}_n$, after subtraction of integers, can always be reduced to one of three possible values $(0, 0)$, $(\bar{1}/3, 0)$ or $(0, \bar{1}/3)$ (Zvyagin, 1967). In the first case, a metrically orthogonal polytype is obtained with $\mathbf{c} \equiv \mathbf{c}_o$; the smallest cell based on the orthohexagonal axes coincides with the orthohexagonal sextuple cell introduced above and is thus a double C-centred cell. For trigonal and hexagonal polytypes, the choice of a primitive hexagonal cell is always possible. The other two cases correspond to non-orthogonal metrically monoclinic polytypes, which can be classified as follows: (i) polytypes with the c axis inclined towards the a axis of the space-fixed reference: these polytypes are grouped under the name *Class a* (b-unique setting); (ii) polytypes with the c axis inclined towards the b axis of the space-fixed reference: these polytypes are grouped under the name *Class b* (a-unique setting). This classification is not simply a matter of names but corresponds to different values of the projection $\mathbf{c}_n$, which is a geometrical feature of non-orthogonal polytypes. The proposed two *Classes* replace the previous definition of $1M$ type and $2M_2$ type (Takeda & Sadanaga, 1969), which is too restrictive,

† The mica real-plane lattice is pseudohexagonal. The effect of the deviation from ideal geometry in phyllosilicates has been studied in detail for kaolin minerals (Zvyagin & Drits, 1996) and seems to influence the formation of different polytypes.

Table 2. *Metrical relations in direct and reciprocal space for both Classes*

	Class a	*Class b*
Direct space	$c\cos\beta = -a/3$	$c\cos\alpha = -b/3$
Reciprocal space	$a^*\cos\beta^* = c^*/3$	$b^*\cos\alpha^* = c^*/3$

because it includes also the definition of the monoclinic angle for all polytypes with $N \neq 3K$ ($K \geq 0$, integer). The metrical relations characterizing these two *Classes*, with respect to the space-fixed reference, are given in Table 2. For polytypes with N and N' layers, the following formulae hold (Zvyagin, 1967):

$$\begin{array}{cc} \textit{Class a} & \textit{Class b} \\ \tan\beta_N = (N/N')\tan\beta_{N'} & \tan\alpha_N = (N/N')\tan\alpha_{N'}. \end{array} \quad (2)$$

In a monoclinic metric, analogous relations hold also for the corresponding angles in the reciprocal space.

As shown by Takeda & Sadanaga (1969), when $N = 3K$ the choice of the axial setting is geometrically limited. For a better understanding of these limitations, it is useful to express the number of layers contained in a repeat unit of each polytype in terms of the powers of 3. The set of positive integers as a function of the powers of 3 assumes the expression:

$$N = 3^n(3K + L) \quad (n \geq 0,\ L = 1 \text{ or } 2). \quad (3)$$

In (3), three characteristic integers are used: n, L and K. It will be shown that n characterizes polytypes that can be based on an axial setting with constant monoclinic angle, whereas L characterizes the transformation rule between different axial settings. Therefore, the following definitions are introduced: *Series*, which corresponds to the number n; and *Subclass*, which corresponds to the number L. The two *Subclasses* 1 and 2 are correspondingly defined. For each *Series*, $K = 0$ of *Subclass* 1 determines the axial setting of the first polytype of the *Series*. This axial setting is called the *basic axial setting* and on it, for each polytype of the *Series*, an axial setting always having the same monoclinic angle can be built.

4. Axial settings

The basal nodes of the C lattice are described by the vector $(p/2, q/2)$, where p and q are coprime integers of the same parity. In the case of non-orthogonal mica polytypes, $\mathbf{c}_n = a/3$ or $b/3$. Therefore, the $\mathbf{c}''_n$ projection of any $\mathbf{c}''$ vector defining C cells of constant volume for those polytypes is obtained adding $(p/2, q/2)$ to $(\bar{1}/3, 0)$ or $(0, \bar{1}/3)$. Using the metrical relation between a and b axes ($b = a \times 3^{1/2}$), the modulus of $\mathbf{c}''_n$ is obtained as follows:

$$\begin{aligned} c''_n/a &= [p^2/4 + 3q^2/4 - (3p-1)/9]^{1/2} \\ c''_n/b &= [p^2/12 + q^2/4 - (3q-1)/9]^{1/2} \end{aligned} \quad (4)$$

for *Class a* and *Class b* polytypes, respectively.

4.1. *Class a*

The monoclinic axial setting of *Class a* having $c_n = a/3$ corresponds to the conventional cell: it will be called the *Standard setting* ($^a\mathbf{S}$). The *alternative setting* will be any other possible C-centred setting. Labelling $^a\mathbf{S}_N$ the standard setting common to all the polytypes with the same number of layers, the basic axial setting for all *Class a* polytypes with $N \neq 0 \pmod 3$ is labelled $^a\mathbf{S}_1$.

4.2. *Class b*

In the case of *Class b* polytypes, the definition of axial settings is a little different. In (1), matrices Π and Π^{-1} have the (13) and (23) elements exchanged because the c axis is inclined towards b and not a. The corresponding transformation:

$$\begin{aligned} &(a\ \ b\ \ c')\Pi = (a\ \ b\ \ c), \\ &\Pi = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \frac{\bar{1}}{3} \\ 0 & 0 & \frac{1}{3} \end{bmatrix}, \quad V = V'/3, \\ &(a\ \ b\ \ c)\Pi^{-1} = (a\ \ b\ \ c'), \\ &\Pi^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 3 \end{bmatrix}, \quad V' = 3V \end{aligned} \quad (1a)$$

leads to an a-unique monoclinic setting. It is common practice to exchange a and b axes (Smith & Yoder, 1956), reverting to a b-unique monoclinic setting. The a-unique setting will be called *Class b Transitional setting* ($^b\mathbf{T}$) and, by analogy with *Class a*, the Standard setting ($^b\mathbf{S}$) will be that deriving from the axial exchange. The $^b\mathbf{T} \rightarrow {}^b\mathbf{S}$ transformation involves the exchanges $a \rightarrow -b$, $b \rightarrow -a$, and $c \rightarrow -c$ in order to resume to a right-handed setting with non-acute β angle, so that this axial transformation is accomplished by the matrix

$$\nabla = \begin{bmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}_{^b\mathbf{T}\rightarrow{}^b\mathbf{S}}, \quad (5)$$

which is an orthogonal matrix, *i.e.* a real and symmetric matrix whose inverse coincides with the matrix itself: $\nabla = \nabla^{-1}$. All the other possible settings with the same $(\mathbf{a}, \mathbf{b})$ basis, are grouped under the definition of alternative settings.

In the case of *Class b* polytypes, there is no 1-layer polytype and the basic axial setting is defined by analogy with *Class a* (Fig. 1). Having already defined $^a\mathbf{S}_1$ setting, its relation to $^a\mathbf{S}_2$ can be derived taking into account that $c_n(2) = c_n(1)$ and $c_o(2) = 2c_o(1)$:

$$(a \quad b \quad c)_{^a\mathrm{S}_1} = (a \quad b \quad c)_{^a\mathrm{S}_2} \begin{bmatrix} \bar{1} & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 \\ 0 & 0 & \frac{1}{2} \end{bmatrix}$$
$$\begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix}_{^a\mathrm{S}_1} = \begin{bmatrix} \bar{1} & 0 & 1 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 2 \end{bmatrix} \begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix}_{^a\mathrm{S}_2}, \qquad (6)$$

i.e. the Standard setting of the simplest polytype belonging to this *Class* ($2M_2$ polytype) is obtained from the C_1 setting through matrices Π and ∇, defined in (1*a*) and (5). The basic axial setting for *Class b* (labelled $^b\mathbf{S}_1$) is obtained by changing the superscript *a* into *b* in (6). The axis a^* of $^b\mathbf{S}_1$ contains the $\bar{2}01$ reciprocal-lattice point (indexing in $^b\mathbf{S}_2$). The geometrical definition of the basic axial settings for the two *Classes* is exactly the same. Taking into account that c_o is the same both in $^b\mathbf{S}_1$ and in $^a\mathbf{S}_1$, while c_n is $-b/3$ in $^b\mathbf{S}_1$ but $-a/3$ in $^a\mathbf{S}_1$, the value of the monoclinic angle of $^b\mathbf{S}_1$ is approximately 107°.

4.3. *Fixed-angle setting for Class a*

The particular alternative setting based on $^a\mathbf{S}_1$, *i.e.* having the same monoclinic angle but $c(N) = Nc(1)$, is defined as the *Fixed-angle setting* ($^a\mathbf{F}_N$). For a 1*M* polytype: $^a\mathbf{S}_1 \equiv {}^a\mathbf{F}_1$. In Fig. 2, the (*h*0*l*) plane of $^a\mathbf{S}$ is shown. The actual values of a^*, c^* and β^* depend on the polytype.

Remembering the metrical relations for *Class a* in reciprocal space (Table 2), the projections on the c^* axis of the vectors $\mathbf{r}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$ are $(3l \pm 2)c^*/3$ so that an integral multiple of c^* is never obtained. The a^* axis of the Fixed-angle setting passes on $\pm 20l$ ($^a\mathbf{S}$ indexing), where the value of l depends on N. Labelling $^o\beta^*_N$ the angle between the c^* and a^* axes of the Fixed-angle setting of an N-layer polytype, the following relationship holds:

$$\tan \beta^*_N(h = \pm 2) = [(3l \pm 2)/2] \tan {}^o\beta^*_N. \qquad (7)$$

Now, putting $N' = 1$ in the reciprocal-space equation corresponding to (2) for *Class a* polytypes, since by definition $\beta^*_1 = {}^o\beta^*_1 = {}^o\beta^*_N$, gives

$$\tan {}^o\beta^*_N = (1/N) \tan \beta^*_N. \qquad (8)$$

Comparison of (8) and (7) gives $N = (3l \pm 2)/2$. The possible solutions are those leading to integral values of l, *i.e*:

$$h = \bar{2} : l = 2K + 2 \quad (\text{for } N = 3K + 2); \qquad h = 2 : l = 2K \quad (\text{for } N = 3K + 1). \qquad (9)$$

No solution can be found for $N = 3K$. Therefore, if and only if $N \neq 3K$, the $^a\mathbf{F}$ setting can be used. The general transformation rule between $^a\mathbf{S}$ and $^a\mathbf{F}$ settings can be obtained by requiring that a^* of $^a\mathbf{F}$ contains the node $h0l$ with

$$h = 2(-1)^{L-1}; \quad l = 2(K + L - 1). \qquad (10)$$

For polytypes belonging to *Subclass* 1 or 2, the $+a^*$ semi-axis of $^a\mathbf{F}$ is respectively in the same or the opposite half-plane containing the $+a^*$ semi-axis of the $^a\mathbf{S}$. It follows that for *Subclass* 2 polytypes $^a\mathbf{S}_N$ is obtained from the basic axial setting ($^a\mathbf{S}_1$, which coincides with $^a\mathbf{F}_1$ and is the basis for obtaining $^a\mathbf{F}_N$), changing sign to *a* and *b* and taking $c(N) = (3K + 2)c_1 + (K + 1)a$. For *Subclass* 1, instead, *a* and *b*

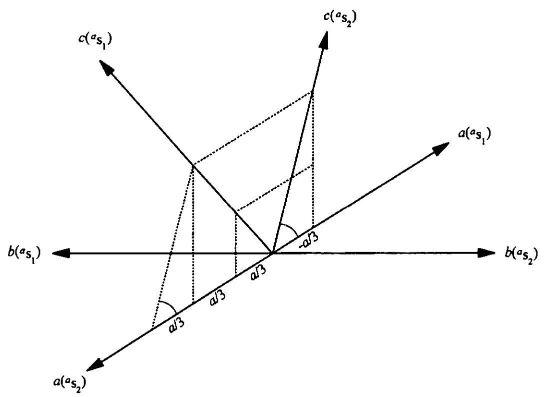

Fig. 1. Geometrical definition of basic axial setting for *Class a* polytypes starting from the Standard setting of the 2-layer polytype ($2M_1$). By exchanging *a* and *b* axes, the same procedure converts the Standard setting of the $2M_2$ polytype into the basic axial setting for *Class b* polytypes.

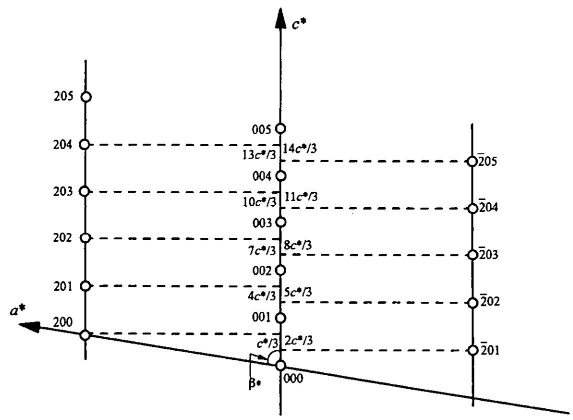

Fig. 2. Definition of Fixed-angle setting for multilayer polytypes. The (*h*0*l*) plane of the $^a\mathbf{S}$ setting is shown, limited to $h = 0$, ± 2 and l from 0 to 5. The projection of reciprocal-lattice nodes on the c^* axis never corresponds to an integral multiple of the period along c^*.

remain unchanged and $c(N) = (3K+1)c_1 + Ka$. In this way, we resume a c_n projection of $-a/3$ ($a/3$ along $+a$ of ${}^a\mathbf{S}_1$ setting for *Subclass* 2, and along $-a$ of the same setting for *Subclass* 1). The ${}^a\mathbf{F}$ setting is based on ${}^a\mathbf{S}_1$ but its c_o is the same as in ${}^a\mathbf{S}_N$ setting. Therefore, the matrix transforming the ${}^a\mathbf{S}$ into ${}^a\mathbf{F}$ does not depend on N. The general expression for the transformation matrices of both *Subclasses*, as a function of K and L, is

$$\Xi_L = \begin{bmatrix} (-1)^{L-1} & 0 & (-1)^L(K+L-1) \\ 0 & (-1)^{L-1} & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (11)$$

It should be noted that $\Xi_1 \neq \Xi_1^{-1}$ and $\Xi_2 = \Xi_2^{-1}$. The matrices accomplishing the transformations from the orthohexagonal space fixed reference are $\Gamma_L = \Pi\Xi_L$.

4.4. *Fixed-angle setting for Class b*

The Fixed-angle setting for this *Class*, ${}^b\mathbf{F}$, is built on ${}^b\mathbf{S}_1$ by taking N times the period along c. As for *Class a*, ${}^b\mathbf{F}$ is not possible for polytypes with a number of layers N that is an integral multiple of three. Starting from ${}^b\mathbf{S}$, the general features of *Class b* polytypes are the same as those of *Class a*. In fact, Fig. 2 and equations (7)–(10) apply also to *Class b* if $a^* < b^*$ is assumed. Furthermore, since the geometrical definition of the basic axial setting is the same for both *Classes*, following the above procedure, identical transformation matrices are obtained. However, the following two facts should be kept in mind: (i) ${}^a\mathbf{S}$ always has a and b axes coincident with those of the space-fixed setting [equation (1)]; (ii) in *Class b*, the setting having a and b coincident with those of the space-fixed setting, is the a-unique setting ${}^b\mathbf{T}$, while the b-unique ${}^b\mathbf{S}$ setting is obtained from ${}^b\mathbf{T}$ through application of the ∇ matrix. The matrix accomplishing the direct transformation from ${}^b\mathbf{T}$ to ${}^b\mathbf{F}$ is

$$^{\nabla}\Xi_L = \nabla\Xi_L = \begin{bmatrix} 0 & (-1)^L & 0 \\ (-1)^L & 0 & (-1)^{L-1}(K+L-1) \\ 0 & 0 & \bar{1} \end{bmatrix}, \quad (12)$$

while for the inverse transformation the matrix is $^{\nabla}\Xi_L^{-1} = \Xi_L^{-1}\nabla$. The overall transformation from the orthohexagonal C_1 setting is obtained through the matrices $^{\nabla}\Gamma_L = \Pi\nabla\Xi_L$ and the correspondent inverse ones.

4.5. *Axial settings for 3K-layer polytypes*

The length of c_n for *Subclass L* in the fixed-angle setting can be calculated from (4), in which $p = (-1)^L 2(K+L-1)$ and $q = 0$ (*Class a*) or $p = 0$ and $q = (-1)^L 2(K+L-1)$ (*Class b*). The result is (a

Table 3. *Basic and Fixed-angle axial settings for N-layer polytypes*

Number of layers		Basic axial setting	Fixed-angle setting	c_n
$3K+1$	$3^0 \pmod 3$	${}^{(a;b)}\mathbf{S}_1$	${}^{(a;b)}\mathbf{F}$	−
$3K+2$	$2\times3^0 \pmod 3$	${}^{(a;b)}\mathbf{S}_1$	${}^{(a;b)}\mathbf{F}$	+
$9K+3$	$3^1 \pmod{3^2}$	${}^{(a;b)}\mathbf{S}_3$	${}^{(3,a;3,b)}\mathbf{F}$	−
$9K+6$	$2\times3^1 \pmod{3^2}$	${}^{(a;b)}\mathbf{S}_3$	${}^{(3,a;3,b)}\mathbf{F}$	+
$27K+9$	$3^2 \pmod{3^3}$	${}^{(a;b)}\mathbf{S}_9$	${}^{(9,a;9,b)}\mathbf{F}$	−
$27K+18$	$2\times3^2 \pmod{3^3}$	${}^{(a;b)}\mathbf{S}_9$	${}^{(9,a;9,b)}\mathbf{F}$	+
$81K+27$	$3^3 \pmod{3^4}$	${}^{(a;b)}\mathbf{S}_{27}$	${}^{(27,a;27,b)}\mathbf{F}$	−
$81K+54$	$2\times3^3 \pmod{3^4}$	${}^{(a;b)}\mathbf{S}_{27}$	${}^{(27,a;27,b)}\mathbf{F}$	+

or b according to the *Class*):

$$c_n = (-K - L/3)(a,b) = -(3K+L)(a,b)/3, \quad (13)$$

where a and b are the lengths of the axes of the space-fixed setting. The projection c_n is thus translationally equivalent to $\pm1/3$ along a or b, where minus and plus signs are respectively for *Subclass* 1 and 2. For $N = 3K$, the Fixed-angle setting cannot be used [equation (9)]; in fact it would have $c_n = -K(a,b)$, translationally equivalent to $(0,0)$. This value is not possible for the non-orthogonal polytypes. However (Fig. 3), the Standard setting of a polytype with 3^n layers (${}^{3^n,a}\mathbf{S}$ and ${}^{3^n,b}\mathbf{S}$) can be used as basic axial setting for polytypes with a number of layers that is a multiple of 3^n, but different from 3^{n+m} or multiple ($m > 0$), exactly in the same way as the 1-layer based setting can be used as basic axial setting for *Class a* polytypes with $N \neq 3$. The resulting fixed-angle settings are labelled ${}^{3^n,a}\mathbf{F}$ and ${}^{3^n,b}\mathbf{F}$, respectively for *Class a* and *Class b*. In this way, the number of

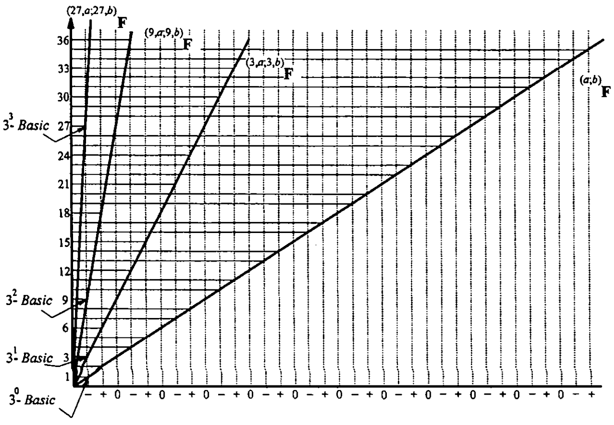

Fig. 3. Definition of Fixed-angle setting for N-layer polytypes. Ordinate: the number of layers. Abscissa: the component of $\mathbf{c}_n$ (along a or b of the space-fixed reference, depending on the *Class*), expressed as −, + and 0. The thick lines represent the c axes of the Fixed-angle settings indicated by the corresponding labels. The intersection of a line parallel to the abscissa with c gives the reduced component of $\mathbf{c}_n$. When this value is zero, the corresponding basic axial setting cannot be used to build a Fixed-angle setting. Note especially settings of polytypes with $N = 0 \pmod 3$

Table 4. *Example of polytype classification according to K, Series and Subclass*

		Series 0	Series 1	*Series* 2	*Series* 3	**S**→**F**
K	*Subclass*	Number of layers	Number of layers	Number of layers	Number of layers	Transformation matrix
0	1	1	3	9	27	Ξ_1
0	2	2	6	18	54	Ξ_2
1	1	4	12	36	108	Ξ_1
1	2	5	15	45	135	Ξ_2
2	1	7	21	63	189	Ξ_1
2	2	8	24	72	216	Ξ_2
3	1	10	30	90	270	Ξ_1
3	2	11	33	99	297	Ξ_2
4	1	13	39	117	351	Ξ_1
4	2	14	42	126	378	Ξ_2
Fixed-angle setting		$^{(a;b)}\mathbf{F}$	$^{(3,a;3,b)}\mathbf{F}$	$^{(9,a;9,b)}\mathbf{F}$	$^{(27,a;27,b)}\mathbf{F}$	

Table 5. *Cell parameters in different axial setting for two polytypes (example)*

The parameters have been calculated assuming ideal parameters for the 1*M* polytype as $a = 5.2$, $b = 9.0$, $c = 10$ Å, $\beta = 100°$. Projection c_n is given making reference to the a and b axes of C_1 setting.

Polytype	Setting	c_n	a (Å)	b (Å)	c(Å)	α (°)	β (°)	a^* (Å^{-1})	b^* (Å^{-1})	c^* (Å^{-1})	α^* (°)	β^* (°)
8 layers,	C_1	(0, 0)	5.2	9.0	236.4	90	90	0.192	0.111	0.00423	90	90
Class a	$^a\mathbf{S}$	($\bar{1}$/3, 0)	5.2	9.0	78.8	90	91.3	0.192	0.111	0.0127	90	88.7
	$^a\mathbf{F}$	(8/3, 0)	5.2	9.0	80.0	90	100	0.195	0.111	0.0127	90	80
11 layers,	C_1	(0, 0)	5.2	9.0	325.1	90	90	0.192	0.111	0.00308	90	90
Class b	$^b\mathbf{T}$	(0, $\bar{1}$/3)	5.2	9.0	108.4	91.6	90	0.192	0.111	0.00923	88.4	90
	$^b\mathbf{S}$	(0, $\bar{1}$/3)	9.0	5.2	108.4	90	91.6	0.111	0.192	0.00923	90	88.4
	$^b\mathbf{F}$	(0, 11/3)	9.0	5.2	113.3	90	107.0	0.111	0.201	0.00923	90	73.0

possible Fixed-angle settings is kept at a minimum (Table 3).

4.6. *Axial transformations*

The consequences of (3) and related definitions can be summarized as follows. The integer n determines the basic axial setting common to all polytypes of the corresponding *Series*, while the *Subclass* defines the direction of the a^* axis of the Fixed-angle setting with respect to that of the Standard setting. All polytypes belonging to a given *Series* can be indexed in their own Standard setting and in the Fixed-angle setting obtained by multiplying by $N/3^n$ the period along c of the corresponding basic axial setting. The transformation matrices between the Standard and the Fixed-angle setting depend on the *Subclass* L and on K. The general transformation rule can be obtained by taking into account the relation between the monoclinic angles of polytypes in (2). For each *Class*, the transformation depends just on the number N of layers in the polytype and on the *Subclass*. If N represents the number of layers of a general polytype and N' the number of layers of the polytype defining the corresponding basic axial setting, by definition, $N = 3^n(3K + L)$ and $N' = 3^n$ hold. Therefore, the ratio

$$N/N' = 3^n(3K + L)/3^n = 3K + L \qquad (14)$$

is completely independent of the *Series*. Polytypes belonging to the same *Subclass* and with the same value of K transform from the Standard setting to the respective Fixed-angle setting exactly in the same way, by means of the same matrix (see Table 4). This result is also independent of the *Class* (if one starts from the standard, and not the transitional setting of *Class b*), since the special features defining a *Class* are contained in the axial parameters and not in the transformation rules. An example of classification is given in Table 4. Cell parameters in the above introduced settings are shown in Table 5 for an 8-layer *Class a* polytype and an 11-layer *Class b* polytype.

5. Discussion and conclusions

Mica polytypes can be divided into orthogonal and non-orthogonal groups. In the case of orthogonal polytypes, the standard ($^{(a,b)}\mathbf{S}$) and fixed-angle ($^{(3^n,a;3^n,b)}\mathbf{F}$) settings coincide; therefore, c coincides with c_o, $\mathbf{c}_n = (0, 0)$ and the choice of the axial setting is simple. However, in the case of orthogonal polytypes and of *Class b* polytypes, additional checks on the space orientation have to be considered, since there are respectively six and three orientations leading to the same projection $\mathbf{c}_n$ (Zvyagin, 1967). This additional check is accomplished by taking into account the symmetry transformation rules among

Table 6. *Features of the axial settings for N-layer mica polytypes*

$a(^a\mathbf{S}) = a(^b\mathbf{T}) = a(^a\mathbf{F}) = a(C_1)$; $a(^b\mathbf{S}) = a(^b\mathbf{F}) = b(C_1)$; $b(^a\mathbf{S}) = b(^b\mathbf{T}) = b(^a\mathbf{F}) = b(C_1)$; $b(^b\mathbf{S}) = b(^b\mathbf{F}) = a(C_1)$.

Orthogonal setting†	$^a\mathbf{S}$ setting/$^b\mathbf{S}$ setting	$^b\mathbf{T}$ setting	$^a\mathbf{F}$ setting	$^b\mathbf{F}$ setting
$\mathbf{c}_n = (0, 0)$	$\mathbf{c}_n = (-1/3, 0)$	$\mathbf{c}_n n = (0, -1/3)$	$\mathbf{c}_n(N) = (-N/3, 0)$	$\mathbf{c}_n(N) = (-N/3, 0)$
$c(N)/c(N') = N/N'$	$c(N)/c(N') = N \sin\beta_N/N' \sin\beta_{N'}$	$c(N)/c(N') = N \sin\alpha_N/N' \sin\alpha_{N'}$	$c(N)/c(N') = N/N'$	$c(N)/c(N') = N/N'$
$\alpha = \beta = 90°$	$\alpha_N = 90°$	$\tan\alpha_N = -3c_o(N)/b$	$\alpha_N = 90°$	$\alpha_N = 90°$
	$\tan\beta_N = -3c_o(N)/a$	$\beta_N = 90°$	$\beta_N = \beta_{1M}$	$\tan\beta_N = \frac{1}{2}\tan\beta_{2M_2}$

† Based on orthohexagonal axes.

Z symbols (Zvyagin, 1974). In the case of non-orthogonal polytypes, the choice of the axial setting is of critical importance, especially when the number of layers increases. The initial transformation from the C_1 setting is accomplished by matrix Π, leading to $^a\mathbf{S}$ [*Class a*: equation (1)] or $^b\mathbf{T}$ [*Class b*: equation (1*a*)] settings; *a* and *b* axes of these two settings always coincide with those of the space-fixed reference. In the other settings, these axes can have the same or opposite orientation with respect to the space-fixed reference, depending on the number of layers, but the Fixed-angle setting for both *Classes* has the same monoclinic angle as the basic axial setting. The general features are summarized in Table 6. In all cases, for two general polytypes with N and N' layers, $c_o(N)/c_o(N') = N/N'$. Therefore, in the $^{(a,b)}\mathbf{S}$ settings, the length c_n is fixed and the monoclinic angle changes with the number of layers. The opposite is true in the $^{(3^n,a;3^n,b)}\mathbf{F}$ settings.

The $^{(a,b)}\mathbf{S}$ settings correspond to the conventional cell and to a projection $\mathbf{c}_n(\bar{1}/3, 0)$, *i.e.* the minimal value for all non-orthogonal polytypes. These settings have thus often been chosen when describing micas (see, for example, Hendricks & Jefferson, 1939; Peacock & Ferguson, 1943; Smith & Yoder, 1956). However, the $^{(3^n,a;3^n,b)}\mathbf{F}$ settings can be singled out using just the *Class* and the number of layers, and the transformations towards the other possible settings are straightforward. For this reason, they have some advantages over $^{(a,b)}\mathbf{S}$, especially when dealing with the reciprocal lattice.

Let the period along c^* for $1M$ polytype be c_1^* (it is about 0.1 Å^{-1}). The diffraction pattern of an N-layer mica polytype shows N spots along any reciprocal-lattice row parallel to c^* within the c_1^* repeat. Some of these spots are ideally absent: they correspond to the additional reflection conditions (as defined in Hahn & Vos, 1983), which can be interpreted in terms of non-characteristic crystallographic orbits (Engel *et al.*, 1984) and by means of the OD theory (Dornberger-Schiff, 1966). However, especially in the case of dioctahedral micas (Takeda & Ross, 1995), where the deviations from the ideal geometry are larger, the additional reflection conditions are violated and the corresponding spots can appear, although with a weak intensity. Because of the large number of reflections, the choice of the correct axial setting is not straightforward, at least with two-dimensional patterns containing the c^* axis. In this case, since, for each *Class* and N, $^{(3^n,a;3^n,b)}\mathbf{F}$ settings are known *a priori*, they are suggested to be, at least initially, used.

5.1. *Applications*

5.1.1. *$4M_3$ polytype*. As an example of application of the diffraction pattern interpretation based on the settings presented in this paper, the case of the $4M_3$ polytype, belonging to *Class a*, *Subclass* 1, and described by Z symbols 3531 and RTW symbols $2\bar{2}\bar{2}2$† is discussed. This polytype was identified by means of oblique-texture electron diffraction (Zhukhlistov *et al.*, 1990). These authors made reference to the orthohexagonal setting, having a repeat of 12 layers along the *c* axis, in which the reflection conditions are given in the synthetic expression

$$k = 3n : l_{12} = 12n \pm 4; \quad k \neq 3n : l_{12} \neq 4n + 2,$$

where l_{12} means that the l index is referred to the 12-layer orthohexagonal unit cell. These synthetic reflection conditions have to be interpreted by taking into account the condition of integrality of monoclinic l indices ($l_{^a\mathbf{S}}$); then, they match the reflection conditions calculated (in the same cell) by means of Zvyagin's functions (Zvyagin, 1967) and shown in the C_1 row of Table 7. By applying matrix Π [equation (1)], the transformation towards $^a\mathbf{S}$ setting implies (h and k unchanged)

$$l_{C_1} = h_{^a\mathbf{S}} + 3l_{^a\mathbf{S}}; \quad l_{^a\mathbf{S}} = (-h_{C_1} + l_{C_1})/3.$$

† Zvyagin's orientation symbols (Z symbols) give the space-fixed intralayer and interlayer displacements in phyllosilicates as a sequence of six digits (1–6) and three symbols (0, +, −), respectively (Zvyagin *et al.*, 1979). However, in the case of micas built by centrosymmetric layers, shortened symbols giving the space-fixed orientation of corresponding layers in a polytype have been introduced (Zhukhlistov *et al.*, 1990): they are written as a sequence of N digits 1–6. RTW orientation-free symbols (Ross *et al.*, 1966) are written as a sequence of N digits 0, ±1, ±2, 3, the jth symbol giving the rotation angle between jth and $(j+1)$th layers as integer multiple of 60°. They can be obtained as the difference between pairs of Z symbols. It is now common practice to include RTW symbols inside square brackets. However, this was not stated by the authors in their original paper (Ross *et al.*, 1966).

Table 7. *Distinctive lattice parameters and reflection conditions for $4M_3$ polytype ($Z = 3531$; $RTW = 2\bar{2}\bar{2}2$) (c_n is referred to a and b axes of C_1 setting)*

a and b are the same as for the $1M$ polytype in all settings. In the ^{a}**F** setting, the reflection conditions assume the simplest expression.

Setting	c_n	β (°)	c (Å)	a^* (Å^{-1})	Reflection conditions
C_1	(0, 0)	90	157.57	0.192	$k = 0 \pmod 3 : l = [12 - 2(h+k)] \pmod{12}$ $k \neq 0 \pmod 3 : l \neq (6 - 8h) \pmod{12}$
^{a}**S**	($\bar{1}$/3, 0)	92.5	39.43	0.192	$k = 0 \pmod 3 : l = h \pmod 4$ $k \neq 0 \pmod 3 : l \neq (h+2) \pmod 4$
^{a}**F**	($\bar{4}$/3, 0)	100	40.00	0.195	$k = 0 \pmod 3 : l = 0 \pmod 4$ $k \neq 0 \pmod 3 : l \neq 2 \pmod 4$

Taking into account the C-centring condition $h + k = 0 \pmod 2$, $l_{^a\mathbf{S}}$ takes the following values (m integer):

$$k = 0 \pmod 3,\ k \text{ even} : h = 2m,\ k = 6m;$$
$$l_{^a\mathbf{S}} = 4 - 6m \pmod 4 = 4 - 3h \pmod 4 = h \pmod 4$$
$$k = 0 \pmod 3,\ k \text{ odd} : h = 2m + 1,\ k = 6m + 3;$$
$$l_{^a\mathbf{S}} = 4 - 3 - 6m \pmod 4 = 4 - 3h \pmod 4 = h \pmod 4$$
$$k \neq 0 \pmod 3 : l_{^a\mathbf{S}} \neq 2 - 3h \pmod 4.$$

Substituting the four possible $h \pmod 4$ values in the last equation, a simpler expression is obtained:

$$k \neq 0 \pmod 3 : l_{^a\mathbf{S}} \neq (h + 2) \pmod 4$$

and the complete expression is as in the ^{a}**S** row of Table 7. Since this example belongs to *Subclass* 1 and corresponds to $K = 1$ [equation (3)], the transformation into the ^{a}**F** setting is accomplished by matrix $\Xi_1(K = 1)$ if starting from ^{a}**S** setting, or by matrix $\Gamma_1(K = 1)$, if starting from C_1 setting. Indices h and k remain again unchanged while the relation between $l_{^a\mathbf{S}}$ (l_{C_1}) and $l_{^a\mathbf{F}}$ is

$$l_{^a\mathbf{F}} = -h + l_{^a\mathbf{S}} \quad [l_{^a\mathbf{F}} = (-4h + l_{C_1})/3].$$

The complete expression of the reflection conditions in the ^{a}**F** setting takes the simplest expression as can be seen in the ^{a}**F** row of Table 7. The axial settings for ($h0l$) and (hhl) planes are shown in Figs. 4 and 5, respectively: the axes of the C_1 setting are fixed, while those of the other two settings can be easily found on the basis of Table 7. Some more examples, including a detailed analysis of the geometrical features of the patterns of 2-layer polytypes ($2M_1$ and $2M_2$) are given in Nespolo *et al.* (1997).

5.1.2. *The PID function.* The most powerful tool to determine the stacking sequences of mica polytypes from diffraction patterns is the periodic intensity distribution (PID) function S^N (Takeda, 1967; Takeda & Sadanaga, 1969; Takeda & Ross, 1995), which represents the Fourier transform of the stacking sequence. The PID is obtained by removing the effect of intensity modulation by the Fourier transform of the single layer from the structure factor. As shown by Takeda & Ross (1995), who adopted the TS unit layers (Takeda & Sadanaga, 1969), the Fourier transform of the stacking sequence can be computed with only the displacements of the TS unit layers in the plane of the layer and without any rotational operation with respect to a given axial setting. For the most common polytypes (those

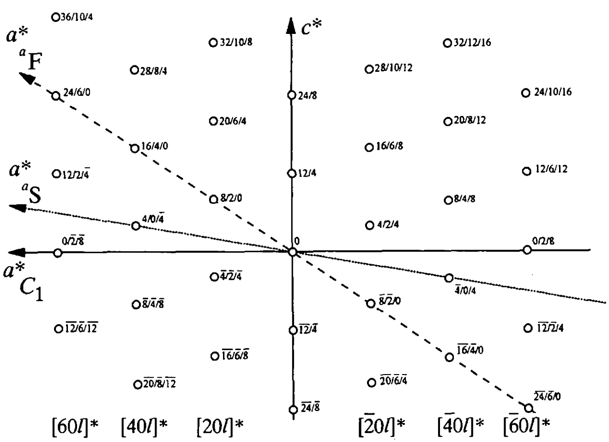

Fig. 4. ($h0l$) reciprocal-lattice plane of $4M_3$ ($Z = 3531$; RTW = $2\bar{2}\bar{2}2$) mica lattice. The scale along c^* and a^* axes is not the same. Indexing: the three numbers represent the l index according to C_1, ^{a}**S** and ^{a}**F**, respectively. For $00l$, indexing according to both ^{a}**S** and ^{a}**F** coincides.

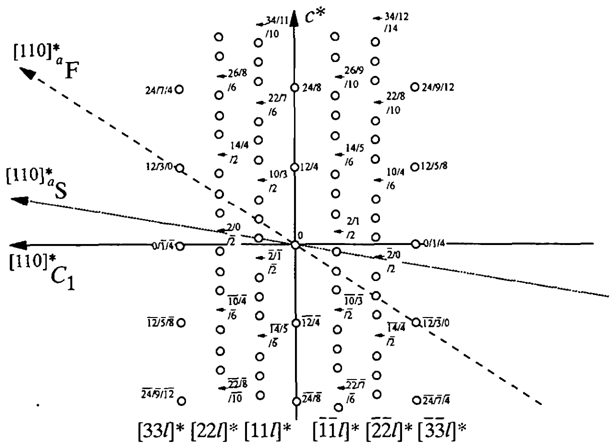

Fig. 5. (hhl) plane of $4M_3$ mica lattice. For explanations, see Fig. 4. Along reciprocal-lattice rows, $h = \pm 3$ nodes corresponding to non-extinguished reflections (one out of four) are indexed, while along the other rows nodes corresponding to extinguished reflections (one out of four) are indexed.

described only by one of the four TS layers), the c axis passing through the origin of each layer is displaced $-a/3$ (*Subclass* 1) or $+a/3$ (*Subclass* 2) for each stacking of layers (Takeda & Ross, 1995). The corresponding axial setting is just the Fixed-angle one. The definition of $^{(3^n,a;3^n,b)}\mathbf{F}$ settings presented in this paper includes and generalizes the criterion used by Takeda & Ross (1995) to all possible polytypes, such as given in their Tables 4, 7, 8 and 10.

Without a common setting, comparisons of the observed and calculated PID in principle have to be repeated $2N$ times, by shifting of the origin and inversion of the sequence. With the $^{(3^n,a;3^n,b)}\mathbf{F}$ settings, the symmetry of the PID function can be expressed with simpler reflection conditions.

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