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## Composite twins of 1M mica: derivation and identification

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### Abstract.

1M is the simplest and one of the most common mica polytypes. Because of the special cell dimensions, twinning by reticular pseudo-merohedry is frequently observed. The possible orientations of the individuals in the twin are approximately the same as the possible orientations of layers in polytypes. Because of the presence of a pseudo-hexagonal twin lattice, five pairs of twin laws are possible and they give rise to five pairs of corresponding twins. Thirty-one composite twins can be enumerated, which however give rise to ten different diffraction patterns. In the twin lattice there are nine geometrically independent rows parallel to  $c^*$ , defining a *minimal rhombus* in reciprocal space, which allows us to identify the ten independent patterns. A larger unit of translation, called *tessellation rhombus*, can be built on it; by tessellation of this unit all the reciprocal space can be covered.

### Introduction.

In Nature, concepts of *complexity* and *simplicity* are often related. Complex natural compounds quite often are made up of one or more simple units, which are arranged in complex ways. Examples are proteins in biology, and mineral polytypes in the inorganic structures. Well before the structural determination of proteins, Ito (1950) reached a simple explanation of the structure of many complex minerals, by applying the idea of *twin of the unit-cell scale*. Group-theoretical treatment for this kind of twins has been developed by Sadanaga (1962, 1963, 1978, 1986). When twinning in a cell scale yields, with concomitant changes in composition, a chemical series of structures, the phenomenon is called “*tropochemical cell-twinning*” (Takéuchi, 1978; Takéuchi, Ozawa and Takagi, 1979; Takéuchi, 1996)<sup>\*1</sup>

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<sup>\*1</sup> The original term “tropochemical twinning” used in Takéuchi (1978) has been modified in the more appropriate “tropochemical cell-twinning” in Takéuchi, Ozawa and Takagi (1979).

Micas compose one of the families in which phyllosilicates are divided and are among the most representative examples of complex structures made up by a single basic structural unit. They display both polytypes and twins as the two faces of having a simple unit, and the relation between them has to be clarified.

As shown by Pabst (1955), the basic structural unit of micas has layer symmetry  $C12/m(1)$  [notation after Dornberger-Schiff (1959), details in Merlino (1990)]<sup>\*2</sup>. This layer can be stacked in different ways (Hendricks and Jefferson, 1939) and if two next layers are related by space group operations a polytype is formed. If crystals are related by a point group operation a twin arises. The azimuthal orientations obtained by application of twin operations or polytype operations are approximately equivalent (Donnay *et al.*, 1964). Therefore, mica twins in a unit cell scale give a diffraction pattern practically not distinguishable from that of a polytype. This type of twins should be treated as polytypes for identification purposes, reserving the concept of twin for crystals large enough to lead to summation and not interference of the waves diffracted by different individuals. However, in principle twinning itself is a phenomenon different from polytypism and the twinning of units smaller than crystallites [the minute forms defined by Vogelsang (1875)] is supposed to influence the formation of different polytypes. Takeda (1995) suggested a possible mechanism in which a small crystal platelet containing stacking faults deposits on the surface of a crystal growing by spiral growth mechanism. The growing spiral would incorporate the platelet and a new ledge, possibly including stacking faults, will produce a stacking sequence which, depending on the nature of the platelet and on its orientation relative to the growing crystal, can be of longer period. The original crystal and the deposited one are just in a twin relation and thus frequency of formation of particular types is fundamental to explain the polytype formation mechanism (Takeda, 1995). The study of twinning in micas is thus important not only for identification purposes, but also for the perspectives that it will lead to a better understanding of the genesis and mechanisms of polytype formation.

### Twins and two-dimensional regular aggregates of crystals.

In twins, a three-dimensional lattice can be exactly or approximately individuated, which is common to all individuals; it is called *twin lattice*. The ratio of the total number of lattice nodes to the number of lattice nodes restored by the twin operation is called *twin index* (t.i.) (Donnay, 1940). *Obliquity* ( $\omega$ ) is the angle between the twin axis (or twin plane) and the closest irrational axis (or plane) that would be perpendicular to a lattice plane (or axis) (Friedel, 1904, 1926). Twinning is thus classified in four types: merohedry (t. i. = 1,  $\omega$  = 0), pseudo-merohedry (t. i. = 1,  $\omega$  > 0), reticular merohedry (t. i. > 1,  $\omega$  = 0) and reticular pseudo-merohedry (t. i. > 1,  $\omega$  > 0) (Friedel, 1904, 1926). The smaller are the obliquity and

<sup>\*2</sup> Actually, a different type of mica exists, based on a non-centrosymmetric layer, with symmetry  $C12(1)$  (Zvyagin *et al.*, 1985; Zhukhlistov *et al.*, 1996). Only a few examples are known until now and they are related to particular genesis conditions. Some ideas to approach the study of such kind of micas are in Zvyagin and Soboleva (1974).

the twin index, the more frequent the twin occurs. For twins with the same index, the smaller is the obliquity, the higher the frequency of occurrence (Donnay, 1940). The geometrical appearance (position of diffraction spots) of the diffraction pattern from twins by merohedry is the same of that from the single individual. Such twins are subdivided into Classes I and II, depending on whether their Laue symmetry is equal to or lower than the lattice symmetry (Catti and Ferraris, 1976). Twins belonging to Class I cannot be distinguished from single crystals, unless anomalous dispersion is taken into consideration. On the other hand, twins belonging to Class II give intensity distributions different from those of a single crystal and thus can be identified (Catti and Ferraris, 1976).

Mica twins have been observed since early times and twin laws for rotation twins of basic polytypes have been studied by several authors (Dana, 1892; Strüver, 1893; Peacock and Ferguson, 1943; Belov, 1947; Federico and Fornaseri, 1952; Sadanaga and Takéuchi, 1961; Franzini and Schiaffino, 1963; Donnay *et al.*, 1964; Rieder, 1970; Takeda, 1977). Nespolo *et al.* (1997) have called attention on the existence of *corresponding twins* (“*macle correspondantes*”), as defined by Friedel (1904). As it will be shown in the next paragraph, mica twin laws can explain twinned crystals in which the individuals are rotated by (approximately)  $n60^\circ$  ( $n$  integer) around  $c^*$ . However, it is not uncommon to meet samples in which individuals are rotated by a different angle. Takéuchi *et al.* (1972) examined the diffraction patterns from about 400 biotite flakes of metamorphic origin and found a series of different angles, the most common of which was  $30^\circ$ . The same angle has been observed by Veblen (1983) and it can be interpreted as resulting from the image sets (as defined by Buerger, 1961) of two two-dimensional hexagonal lattices (Takéuchi *et al.*, 1972) and by application of the compound tessellation theory (Coxeter, 1973, 1989; Takeda and Donnay, 1965a). Veblen (1983) has called such aggregates of crystals “*chemical twins*”, an expression meaning that some chemical rearrangement occurs in the region close to the contact plane (Andersson and Hyde, 1974; Veblen, 1991). In case of micas, parts of the interlayer cations would be lost, due to the lack of space in the interlayer sites, but this would not alter the chemical formula, unless the “*chemical twinning*” affect many planes (Veblen, 1983). However, as shown by Takéuchi *et al.* (1972), the twin lattice for crystals rotated by  $30^\circ$  should be based on an extremely large two-dimensional mesh; it follows that the twin index would be not realistic. The diffraction patterns showing mica lattices rotated by  $30^\circ$  should be interpreted as *two-dimensional regular aggregates*, instead of twins, and the two-dimensional lattice in the plane of contact can be explained by application of a “pseudo-compound tessellation” (Sueno *et al.*, 1971). It is plausible that in such aggregates a structural control plays a significant role (Wilman, 1951). This topic will be the object of a future publication.

### **Twin laws for 1M mica.**

1M is the simplest of mica polytypes. It is the most common polytype in the trioctahedral sub-family, and it is not uncommon also in the dioctahedral one (Bailey, 1984).

In the plane of the layer, the two monoclinic axes of 1M mica closely follow the metri-

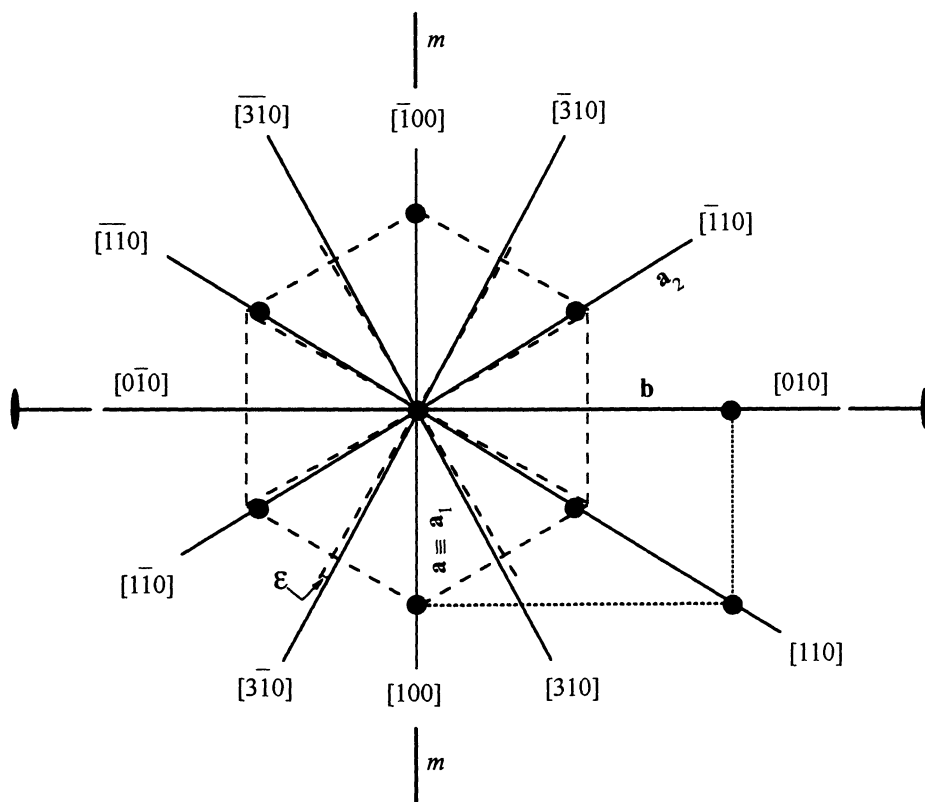


FIG. 1. The five directions in the monoclinic (001) plane which can act as reticular pseudo-merohedry twin axes and planes for 1M mica (solid lines). Dashed lines show the correspondent hexagonal directions, together with the (001) projection of the triple cell obtained by juxtaposing three hexagonal primitive cells. Dotted lines show the sextuple cell in (001) projection. The amount of the deviation from hexagonality, measured by the parameter  $\epsilon$ , is exaggerated because of drawing necessities.

cal relation defining orthohexagonal axes,  $b = a\sqrt{3}$ . The monoclinic  $C$ -centered double cell built on them corresponds to the so-called *conventional cell* (Burzlaff, Zimmermann and De Wolff, 1983). Taking three times the period along  $c$ , an orthogonal, pseudo-orthohexagonal cell can be chosen (Zvyagin, 1967), which represents the unit cell of the twin lattice (Donnay *et al.*, 1964). It is a sextuple cell, whose nodes at height different from  $z = 0$  are not restored by the twin operations. By considering only the nodes on the corners and centering the  $C$  face of the sextuple cell, the twin lattice (pseudo-hexagonal) is obtained and twin index is 3.

Fig. 1 shows the directions of the two-fold axes in an ideal hexagonal two-dimensional lattice and the corresponding directions in the mica monoclinic lattice. The [010] direction, along which is the only two-fold symmetry axis for the structure, is the only direction nor-

TABLE 1. The five pairs of twin laws for 1M mica and their alternative description (orthohexagonal indices)

Twin law (rotation twins)	Rotation around $\mathbf{c}^*$	Twin law (reflection twins)	Rotation around $\mathbf{c}^*$
$[310]_{\pi}$	$240^{\circ}-2\epsilon$	(110)	$240^{\circ}+2\epsilon$
$[110]_{\pi}$	$300^{\circ}-2\epsilon$	(130)	$300^{\circ}+2\epsilon$
$[\bar{3}10]_{\pi}$	$120^{\circ}+2\epsilon$	( $\bar{1}10$ )	$120^{\circ}-2\epsilon$
$[\bar{1}10]_{\pi}$	$60^{\circ}+2\epsilon$	( $\bar{1}30$ )	$60^{\circ}-2\epsilon$
$[100]_{\pi}$	$180^{\circ}$	(100)	$180^{\circ}$

mal to a lattice plane, (010), which in turn is the only symmetry plane for the structure. The other five directions are at  $(n30\pm\epsilon)^{\circ}$  from [010], where  $n = 1, 2, \dots, 5$ . The angle  $\epsilon$  is a measure of the deviation from hexagonality and is related to the obliquity of the twin lattice (Friedel, 1904); it varies between  $10''$  and  $1'$  for  $n \neq 3$ , while it is zero for  $n = 3$  (Donnay *et al.*, 1964), because of the monoclinic lattice. The five directions  $[310]$ ,  $[\bar{3}10]$ ,  $[110]$ ,  $[\bar{1}10]$ ,  $[100]$  are *quasi*-normal to lattice planes and are pseudo-symmetry axes for the multiple, pseudo-hexagonal lattice mentioned above. They can thus act as twin elements by reticular pseudo-merohedry (Friedel, 1904; 1926), giving rise to rotation twins. In their turn, the lattice planes *quasi*-normal to these directions are pseudo-symmetry planes for the multiple, pseudo-hexagonal lattice and they too can act as twin elements by reticular pseudo-merohedry, giving rise to reflection twins. These rotation and reflection twins are not equivalent and have been called *corresponding twins* (Friedel, 1904): they would become equivalent if  $\omega = 0$ . There are thus *five pairs* of twin laws for 1M mica. The five rotation twin laws, each pre-multiplied by a  $180^{\circ}$  rotation around [010], can be described as  $(n60\pm 2\epsilon)^{\circ}$  rotations around  $\mathbf{c}^*$  (Donnay *et al.*, 1964), where upper and lower signs are for  $n = 1, 2$  and for  $n = 4, 5$  respectively; similarly, the five reflection twin laws, each pre-multiplied by a reflection across (010), can be described as  $(n60\pm 2\epsilon)^{\circ}$  rotations around the same axis (Nespolo *et al.*, 1997) (Table 1). The opposite sign of the  $\epsilon$  parameter is due to the non-orthogonality between axes and planes. Hereafter, rotations in direct space are assumed counterclockwise.

The twin reciprocal lattice corresponds to the overlapping of the reciprocal lattice of the individuals building the twin (Buerger, 1954). The twin reciprocal lattice rows which are parallel to  $\mathbf{c}^*$  are called *composite rows* (Sadanaga and Takéuchi, 1961) and show overlapping of nodes depending on the twin law. In this paper it will be shown that a set of composite rows called *geometrically independent rows* are necessary and sufficient to describe the distribution of nodes in reciprocal space for all twins of 1M individuals.

### Geometrically independent rows.

Hereafter, both the single-crystal lattice and the twin lattice are referred to the axial setting of the (pseudo)-orthohexagonal cell mentioned above. The axial setting of the twin lattice is space-fixed; the individuals building the twin are assumed oriented in such a way that the axial setting of the first crystal coincides with that of the twin lattice. Both single-crystal rows

TABLE 2. RS of 1M reciprocal lattice rows.

row	$h \pmod{3}^*$	$k \pmod{3}$	Rotationally related rows	RS
S	0	0	SSSSSS	000000
D <sub>1</sub>	1	0	D <sub>1</sub> D <sub>2</sub> D <sub>1</sub> D <sub>2</sub> D <sub>1</sub> D <sub>2</sub>	121212
D <sub>2</sub>	2	0	D <sub>2</sub> D <sub>1</sub> D <sub>2</sub> D <sub>1</sub> D <sub>2</sub> D <sub>1</sub>	212121
X <sub>1</sub>	1	1	X <sub>1</sub> X <sub>4</sub> X <sub>3</sub> X <sub>2</sub> X <sub>5</sub> X <sub>6</sub>	110220
X <sub>2</sub>	2	2	X <sub>2</sub> X <sub>5</sub> X <sub>6</sub> X <sub>1</sub> X <sub>4</sub> X <sub>3</sub>	220110
X <sub>3</sub>	0	1	X <sub>3</sub> X <sub>2</sub> X <sub>5</sub> X <sub>6</sub> X <sub>1</sub> X <sub>4</sub>	022011
X <sub>4</sub>	1	2	X <sub>4</sub> X <sub>3</sub> X <sub>2</sub> X <sub>5</sub> X <sub>6</sub> X <sub>1</sub>	102201
X <sub>5</sub>	2	1	X <sub>5</sub> X <sub>6</sub> X <sub>1</sub> X <sub>4</sub> X <sub>3</sub> X <sub>2</sub>	201102
X <sub>6</sub>	0	2	X <sub>6</sub> X <sub>1</sub> X <sub>4</sub> X <sub>3</sub> X <sub>2</sub> X <sub>5</sub>	011022

\* in the single-crystal,  $l \pmod{3} = h \pmod{3}$

and composite rows are defined by their reciprocal lattice nodes with indices of  $(h, k)$  (Table 2).

Since 1M mica twinning is by reticular pseudo-merohedry, the rows parallel to  $\mathbf{c}^*$  of the individuals overlap only approximately in the twin lattice and, in principle, nodes on composite rows actually occupy very close but distinct positions. However, because of the physical (non-zero) dimension of the diffraction spots, no perceivable splitting is expected to be normally recorded. For this reason, the parameter  $\varepsilon$  can be taken as zero for the present purpose. This means that practically twin operations can be described as  $n60^\circ$  rotations around  $\mathbf{c}^*$ , which correspond to the linear part of the space group operations relating layers in mica polytypes. Therefore, the six possible approximated orientations of crystals in 1M twins are the same as the six possible exact orientations of layers in mica polytypes.

The reciprocal lattice of 1M mica polytype shows one node in the period along  $\mathbf{c}^*$  (about  $1/10 \text{ \AA}^{-1}$ ) of the conventional cell (hereafter indicated as  $c^*_1$ ), whose inclined  $\mathbf{a}^*$  axis obeys the cell relation  $a^* \cos \beta^* = c^*/3$ . The reciprocal orthohexagonal cell period along  $\mathbf{c}^*$  is  $c^*_1/3$  and within a  $c^*_1$  repeat the values of the  $l$  index are 0, 1 or 2 ( $\pmod{3}$ ), with the constraint  $l = h \pmod{3}$  (Fig. 2).

Counterclockwise rotations in direct space correspond to clockwise rotations in reciprocal space. Six rows are related by the rotations around  $\mathbf{c}^*$ , which (approximately) describe the twin operations. The set of the six  $l \pmod{3}$  values of the nodes belonging to single-crystal reciprocal lattice rows related by clockwise rotations define a *Rotational Sequence* (RS). One RS corresponds to each  $(h, k)$  row; the  $n$ -th digit of a RS corresponds to the  $l$  index of the node on the row which is related to  $(h, k)$  by  $n60^\circ$  clockwise rotation. By analyzing how single-crystal rows transform under  $n60^\circ$  rotations and their corresponding RS, three types of rows can be identified: the twin operations always relate only rows of one and the same type.

1.  $h = 0 \pmod{3}$  and  $k = 0 \pmod{3}$ . All rows of this type have reciprocal lattice nodes at  $l = 0 \pmod{3}$  and there is only one RS (Table 2). Since there is only one geometrically independent row like this, it will be called **S** (for "Single");
2.  $h \neq 0 \pmod{3}$  and  $k = 0 \pmod{3}$ . Rows belonging to this type have reciprocal lattice nodes at  $l = 1 \pmod{3}$  or  $l = 2 \pmod{3}$  but not at  $l = 0 \pmod{3}$  and there are two RS (Table 2).

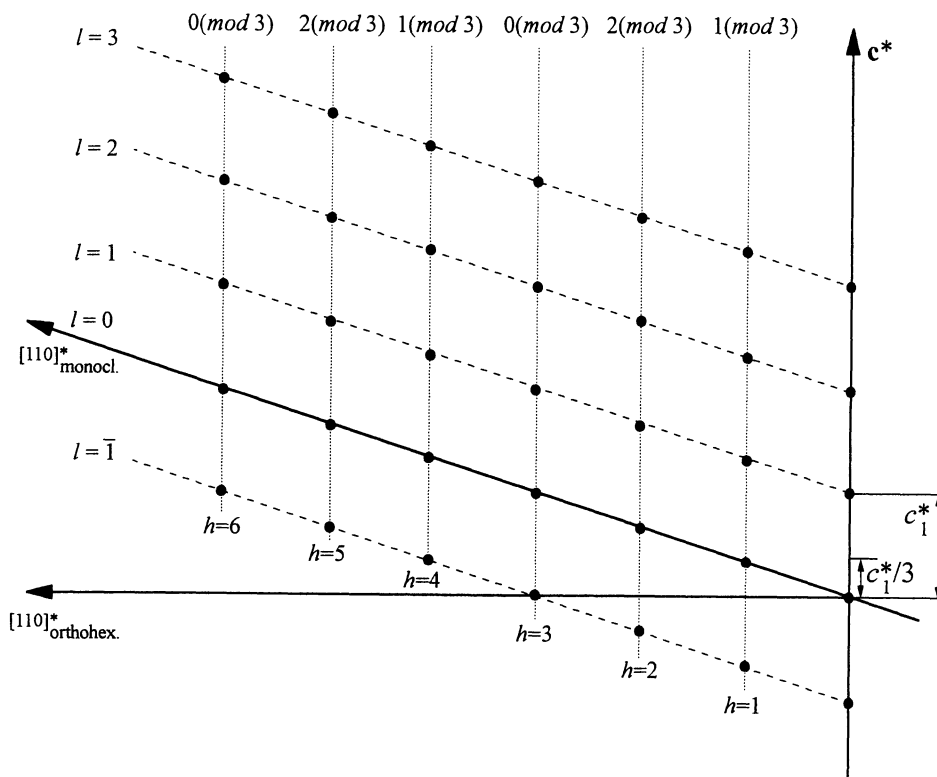


FIG. 2. The  $(11l)$  plane of 1M mica indexed in the monoclinic (indices on the left) and in the orthohexagonal (indices on the top) axial settings. The latter clearly shows the relation  $l = h \pmod{3}$ .

For this reason, this type of row will be called **D** (for “Double”) and subdivided into two geometrically independent rows  $D_j : h = j \pmod{3}, k = 0 \pmod{3} [j = 1, 2]$ ;

3.  $k \neq 0 \pmod{3}$ . Rows belonging to this type have reciprocal lattice nodes at the three possible values of  $l \pmod{3}$  and there are six RS (Table 2). For this reason, this type of row will be called **X** (for “seXtuple”) and subdivided into six geometrically independent rows  $X_j : h = j \pmod{3}, k = [2 \cdot (-1)^j] \pmod{3} [j = 1-6]$

There are thus nine geometrically independent rows by which all the reciprocal space can be described.

### Tessellation rhombus and minimal rhombus.

The difference between the  $(h, k)$  coordinates of two geometrically equivalent rows (two S rows; two  $D_j$  or two  $X_j$  rows with the same  $j$  value) can always be reduced to  $(3p, 3q)$ ,  $p$  and  $q$  integers of the same parity. Therefore, a  $(3p, 3q)$  translation in the  $(\mathbf{a}^*, \mathbf{b}^*)$  plane



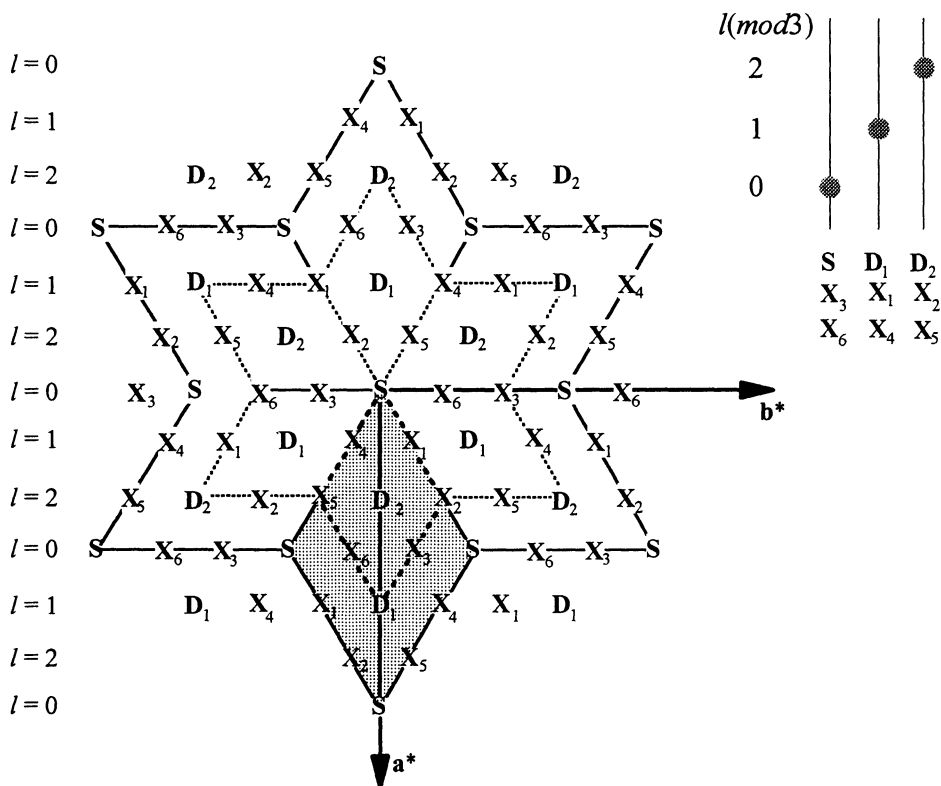


FIG. 3. Definition of minimal rhombus (dotted lines; in the foreground) and tessellation rhombus (solid lines). The two D and the six X geometrically independent rows are distinguished by sequence numbers (D<sub>1</sub> and D<sub>2</sub>; X<sub>1</sub> ~ X<sub>6</sub> respectively). Inset on the upper right:  $l \pmod{3}$  index of the node on single-crystal reciprocal lattice rows.

relates two geometrically equivalent rows. The nine geometrically independent rows form a unit, which in (001) projection has the shape of a rhombus: it is called *tessellation rhombus* (Fig. 3, solid lines). It has S rows at the four vertices (the two S rows at the vertices of the long diagonal belong to six adjacent rhombi; the two S rows at the vertices of the short diagonal belong to three adjacent rhombi), D rows on the long diagonal, inside the rhombus, two X rows inside the rhombus and eight X rows on the edges (they belong to two adjacent rhombi). By  $(3p, 3q)$  translations of the *tessellation rhombus* all the reciprocal space can be tessellated. Inside the *tessellation rhombus*, a smaller unit, called *minimal rhombus*, defined by the same nine geometrically independent rows, can be found (Fig. 3, dotted lines). S and D rows are on the long diagonal, while the six X rows are on the edges. The *minimal rhombus* can be thought of as the asymmetric unit of the *tessellation rhombus*. The distribution of nodes along the nine rows of a *minimal rhombus* is the information needed sufficient to

derive and identify twins. Taking the S row as common origin, there are six distinct orientations of both the *tessellation rhombus* and the *minimal rhombus*, related by  $n60^\circ$  rotations. By effect of these rotations, within a rhombus only the positions of rows belonging to the same type are exchanged (Fig. 3).

The derivation of the independent *twin minimal rhombi* is accomplished as follows:

1. the *individual minimal rhombi* are rotated by  $n60^\circ$  and overlapped;
2. two composite *minimal rhombi* obtained in the previous step are equivalent if the distribution of composite rows on them becomes identical through a  $n60^\circ$  rotation around  $c^*$ .

By definition, in a twin two individuals cannot be oriented in the same way (if so they would just represent a parallel growth of two crystals); therefore, in  $n60^\circ$ :  $n > 0$ . This restriction is not valid for polytypes and thus the number of possible composite twins with a given number of individuals is much smaller than the number of possible polytypes with the same number of layers. In a twin built by  $m+1$  individuals, ( $m = 1 \sim 5$ ),  $n_j$  expresses the rotational relation between the first and the  $(j+1)$ -th individuals, ( $j = 1 \sim m$ ;  $n_j = 1 \sim 5$ ). The number of possible patterns is thus:

$$\sum_{m=1}^5 \frac{5!}{m!(5-m)!} = 31 \quad (1)$$

The resulting patterns of rows can be obtained in the following way. A twin containing  $m+1$  individuals is labelled by a sequence of  $m$  increasing values  $n_j$ . The  $m+1$  rows from the  $m+1$  individuals give rise to a single composite row; the  $l$  index of the node on the  $(j+1)$ -th single-crystal row corresponds to the  $(n_j+1)$ -th value of the RS. The first value of the RS has always to be added; it corresponds to the node from the first individual, with space-fixed ori-

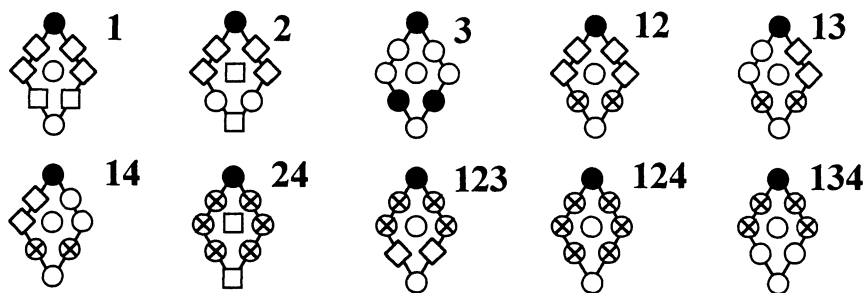


FIG. 4. Identification of 1M twins by means of their minimal rhombi. The rotation angles between successive individuals are indicated as successions of  $n_j$  symbols (see text). Inset on the lower right:  $l \pmod{3}$  indices of the nodes on reciprocal lattice composite rows.

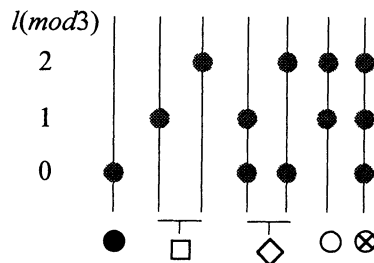


TABLE 3. Composite  $1M$  twins and independent patterns arising from them. The sequence of  $n_j$  represents the rotation angles ( $\text{mod } 60^\circ$ ) between the first and the  $(j+1)$ -th individuals building the twin ( $j = 1 \sim m$ ). These sequences are used to label the twins.

$m$	$n_j$ sequence	Pattern equivalent to	$m$	$n_j$ sequence	Pattern equivalent to
1	1	Unique	3	123	Unique
	2	Unique		124	Unique
	3	Unique		125	123
	4	2		134	Unique
	5	1		135	124
2	12	Unique	145	123	
	13	Unique	234	124	
	14	Unique	235	134	
	15	12	245	124	
	23	14	345	123	
	24	Unique	4	1234	124
	25	13		1235	124
	34	13		1245	124
	35	14		1345	124
	45	12		2345	124
			5	12345	124

entation. The patterns obtained in this way (Fig. 4) show that only ten of the 31 possible ones correspond to different twin *minimal rhombi* (Table 3, Fig. 4).

On composite reciprocal lattice rows up to three nodes can be present within  $c^*_1$ , distributed on the three positions  $l = 0, 1, 2 \pmod{3}$  and the number of composite rows is:

$$\sum_{i=1}^3 \frac{3!}{i!(3-i)!} = 7 \quad (2)$$

However, it can be shown that a less detailed classification in five rows, grouped according to the presence or absence of  $l = 0 \pmod{3}$  node, is sufficient to achieve the highest degree of distinction between the patterns of  $1M$  twins (Fig. 4). The most detailed possible separation into seven rows does not differentiate any additional pattern.

### Application.

One practical example of application of the present approach can be given on the basis of the twin observed by Takeda and Donnay (1965b), who reported a twinned lithium  $1M$  mica, giving the following presence criteria: “for H and K = 0 mod. 3, L = 0 mod. 3; for H = 0 with K  $\neq$  0 mod. 3, L = 0 mod. 3 and L = 1 or 2 mod. 3; for H = 1 or 2 with K = 0 mod. 3, L = 1 and 2 mod. 3; for all others, no conditions. The edifice can be interpreted as a twin of four crystals[...]; the twin operations are  $[100]_{180^\circ}$ ,  $[310]_{180^\circ}$ ,  $[110]_{180^\circ}$ ”.

In the terminology introduced here, the presence criteria given by Takeda and Donnay (1965b) become:

S rows:  $l = 0 \pmod{3}$

$D_1$  and  $D_2$  rows:  $l = 1, 2 \pmod{3}$

$X_1, X_2, X_4, X_5$ :  $l = 0, 1, 2 \pmod{3}$

$X_3, X_6$ :  $l = 0, 1 \pmod{3}$  or  $l = 0, 2 \pmod{3}$ .

Looking at Fig. 4, these conditions correspond to the twin labelled 123. This is a twin composed by four individuals, where the (approximate) rotations around  $\mathbf{c}^*$  with respect to the first individual, having fixed orientation, are  $60^\circ$ ,  $120^\circ$  and  $180^\circ$ . Through the correspondences given above, these approximate rotations are equivalent to  $180^\circ$  rotation around respectively [110], [310] and [100]. Our approach is thus completely consistent with the experimental data and previous interpretation. Furthermore, it is valuable for its complete generality and systematic nature.

### Discussion.

Sadanaga and Takéuchi (1961) took into account only twins in which one and the same twin law is operating, because they were interested in polysynthetic twinning. They classified composite rows into three types, called S, Twin and T. This division corresponds to the present classification in S, D and X, and the  $h$  and  $k$  values also correspond. However, Sadanaga and Takéuchi (1961) classification was based on the number of nodes along the composite rows, and not on a transformation criterion. The definition given in this paper derives from the combination of the two-dimensional (pseudo)-hexagonal symmetry with the cell relation  $l = h \pmod{3}$  and it is thus applicable also to other polytypes that share the same geometrical features (Nespolo, Takeda, Ferraris, in preparation).

Rieder's (1970) analysis grouped together composite rows on which only one node appears ( $l = 0$  or  $1$  or  $2$ ) and rows with two nodes ( $l = 0, 1$  or  $0, 2$  or  $0, 3$ ), thus allowing the recognition of only eight of the ten patterns<sup>\*3</sup>.

Both these previous treatments adopted a twin-related pair of axes  $\mathbf{a}^*$ ,  $\mathbf{b}^*$ , by means of which a correlation with mica polytypes was suggested. Although the linear part of the operator generating twins and polytypes is (approximately) the same, polytypes are generated by space-group operations, while twins by point-group operations and the orientation of the twin lattice should be kept fixed in the space. All the information needed to classify 1M twins are contained in the minimal rhombus. It is just this rhombus that can be rotated in the six possible orientations, in order to compare the calculated pattern with the experimental ones, which have been obtained with an arbitrary orientation of the crystal-fixed reference.

### Conclusions.

In this paper a new approach to derive and identify diffraction patterns of twins on the

<sup>\*3</sup> Rieder tried to differentiate some of the equivalent patterns by considering the angles in the  $h0l$  and  $h.3h.l$  planes of the monoclinic setting. This procedure doesn't lead to a new pattern, while the present detailed classification of composite rows actually individuates different patterns that are treated as identical by Rieder's approach.

basis of the lattice geometry has been presented. It has been successfully applied for twin analysis of a lithium mica. A comprehensive understanding of the geometrical features of crystal and twin lattices is necessary also for a better understanding of the formation of polytypes. In fact, the principles of both the perfect and faulted matrix in the spiral growth around a screw dislocation have revealed that they are able to explain formation of only a part of the observed polytypes (Baronnet and Kang, 1989). The deposition of a new platelet on the surface of a crystal growing by spiral growth (Takeda 1995; Takeda and Ross, 1993) seems able to further explain observed polytypes. Between the growing crystal and the deposited platelet with stacking faults there is an epitaxial relation that can be described in terms of twin laws. The study of twinning is thus of fundamental importance also to understand formation mechanisms.

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