$2^k k!$, with the understanding that for, say, $m = 0$ (5) reduces to $(2n-1)!!/(2n)!!$

The above procedure can readily cope with the calculation of $\langle|J|^4\rangle$ and $\langle|J|^6\rangle$ for any space group. This symbol-handling procedure is also much faster than the first one. Thus, the values of $\langle|J|^4\rangle$ and $\langle|J|^6\rangle$ for the cubic system, the most complex one, including separate calculations for the various *hkl* subsets, have been obtained in less than $1\frac{1}{2}$ min on a CDC6600. However, when the trigonometrical forms given for A and B need extensive rearrangements (*e.g.* for trigonal and hexagonal systems), the structure-factor algebraic procedure described above is preferable in practice.

Results

The fourth and sixth moments of the trigonometric structure factor were computed for all 230 space groups and the results are summarized in Table 1.

Since the symmetry-dependent coefficients required for the evaluation of moments and distributions of the normalized structure factor depend on the ratios q/p^2 and r/p^3, where $p = \langle|J|^2\rangle$, $q = \langle|J|^4\rangle$, $r = \langle|J|^6\rangle$ (Shmueli & Wilson, 1981), and these ratios, rather than the individual moments, are likely to be of use, the results are presented in their terms. Of course, q and r can be readily found since p is given for each entry.

It was assumed throughout the calculation that all the atoms occupy general positions and all the subsets of *hkl* (except those corresponding to zones and rows), giving rise to different functional forms of A and B, were considered. The absence of any remark beside an entry in Table 1 means that all the space groups and/or all the above mentioned subsets of *hkl* corresponding to this entry lead to identical values of p, q and r.

In the comparison of our results for q with those obtained by Wilson (1978) it is appropriate to point out that his results were obtained without the aid of a computer and that the possibility of his tables containing some errors was emphasized (*cf.* §1.7; Wilson, 1978). The comparison showed a single numerical discrepancy ($I4_1/a$), one inconsistent association of a q value with an *hkl* subset ($P4_132$) and two more q values for $P4_132$ not given by Wilson (1978). Also Wilson's values of q for $I4_132$, $I\bar{4}3d$ and $Ia3d$, unlike the other entries in his Table 3 (Wilson, 1978), are not the average q values but coincide with ours for the '*hkl* all even' case. For all the rest, there is an exact agreement regarding q values for primitive space groups and average q values for the centered ones. The values of q for the space groups $Fd3m$ and $Fd3c$, not given by Wilson (1978), were supplied in this work.

Corresponding results for the eighth moment of $|J|$ can now also be computed and will be reported later.

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Stacking Faults and Twins in Kyanite, Al_2SiO_5

BY A. LEFEBVRE AND D. MÉNARD*

Université des Sciences et Techniques de Lille, Laboratoire de Structure et Propriétés de l'Etat Solide, Bâtiment C6, 59655 Villeneuve d'Ascq CEDEX, France

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Abstract

Two types of twins are frequently found in naturally and experimentally deformed kyanite. Structural models based on periodic shears are proposed to account for these mechanical twins. The structure of kyanite is then regarded as layered, the limits of each layer being easy glide planes for dislocations. The shear plane is (100). The shear vectors are $\frac{1}{2}$ [001] and $\frac{1}{2}$ [011]. They are suitable for the only known glide system (100) [001].

* Present address: Service Thermique, DERC Ferodo, 4, rue Gambetta, 93406 St Ouen, France.

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Introduction

Twins in kyanite have been known by mineralogists for a long time [see, for instance, Deer, Howie & Zussman (1978) and Table 1]. Although two of them (α and γ) were found in experimentally deformed samples (Boland, Hobbs & MacLaren, 1977) these twins have not yet been studied by electron microscopy and no structural model has been produced to account for them; that is the intention in this paper.

Table 1. *Twins in kyanite*

Twins	Twinning operations
α	Diad rotation about [001]
β	Diad rotation about [010]
γ	Reflection across (100)

Crystallography of kyanite

The structure of kyanite was determined by Náray-Szabó, Taylor & Jackson (1929) and then refined by Burnham (1963); it is triclinic with space group $P\bar{1}$. This structure can be described in two different ways.

(*a*) *Ionic approach* (*Bragg & West*, 1927)

It can be considered as a slightly distorted f.c.c. oxygen sublattice with Al^{3+} cations in octahedral interstices and Si^{4+} cations in tetrahedral interstices. Leaving aside the triclinic distortion of the oxygen sublattice, we find that the orientation relationship between the vectors $\mathbf{a}_t$, $\mathbf{b}_t$ and $\mathbf{c}_t$ of the triclinic unit cell and the vectors $\mathbf{a}_c$, $\mathbf{b}_c$ and $\mathbf{c}_c$ of the oxygen sublattice unit cell is as follows:

$$\begin{bmatrix} \mathbf{a}_t \\ \mathbf{b}_t \\ \mathbf{c}_t \end{bmatrix} = \begin{bmatrix} 3/2 & \bar{1}/2 & 1 \\ 0 & 2 & 0 \\ \bar{1} & 0 & 1 \end{bmatrix} \begin{bmatrix} \mathbf{a}_c \\ \mathbf{b}_c \\ \mathbf{c}_c \end{bmatrix}.$$

(*b*) *Covalent approach* (*Náray-Szabó et al.*, 1929)

The structure of kyanite is characterized by chains of AlO_6 edge-sharing octahedra extending parallel to the *c* axis. These chains are linked by AlO_6 octahedra and SiO_4 tetrahedra (Fig. 1). They are of special interest because similar arrangements are found in the other two Al_2SiO_5 polymorphs, andalusite and sillimanite.

Experimental

Kyanite crystals from Lesotho xenolithic eclogites and a quartzo feldpatic gneiss (Brioude, Massif Central, France) were used. Thin foils suitable for transmission electron microscopy were prepared by ion bombardment.

Two types of planar stacking faults were commonly observed in the vicinity of twins. They are parallel to (100). The displacement vectors are $\frac{1}{2}[001]$ and $\frac{1}{2}[011]$. The $\frac{1}{2}[001]$ stacking faults correspond to the $[001] \rightarrow \frac{1}{2}[001] + \frac{1}{2}[001]$ dissociation of **c** dislocations found by Boland *et al.* (1977) and Ménard, Doukhan & Paquet (1977). Fig. 2 shows $\frac{1}{2}[011]$ stacking faults with

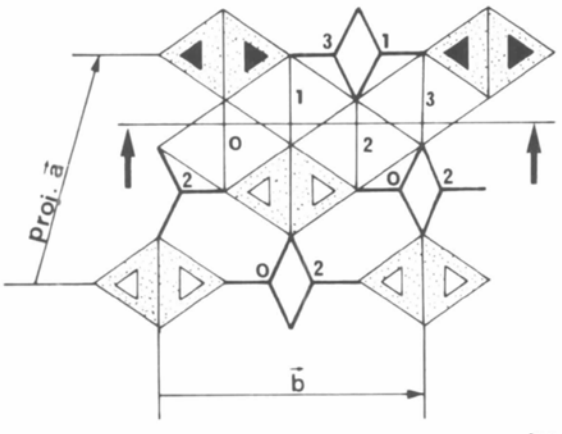

Fig. 1. Idealized projection of kyanite on a plane normal to [001]. AlO_6 chains parallel to [001] are shown as stippled octahedra: the heights of the Al ions in these chains are 0 and $c/2$ (black triangles) or $c/4$ and $3c/4$ (white triangles). The heights of the ions in the other polyhedra are given as multiples of $c/4$: ◁▷ AlO_6 octahedra; —≺ SiO_4 tetrahedra. The easiest glide plane in the cell is arrowed.

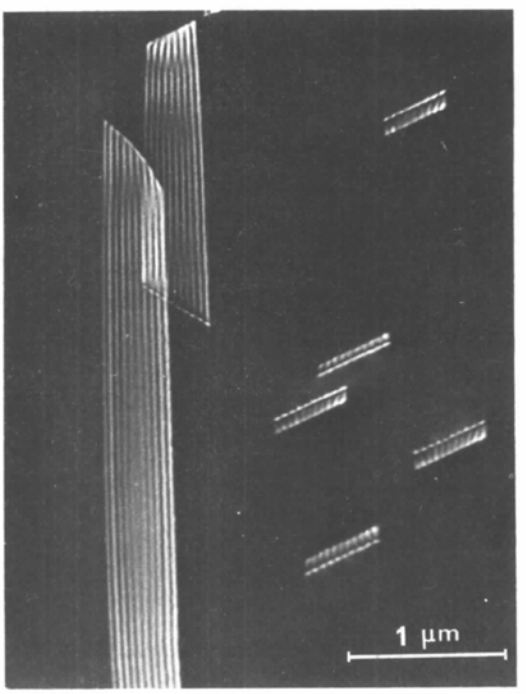

Fig. 2. $\frac{1}{2}[011]$ stacking faults in Lesotho kyanite. Weak beam, $g = 030$.

lengths that can be very different. The two partial dislocations bounding each fault have different contrast, which indicates that they have different Burgers vectors; these vectors have not yet been clearly identified. They probably correspond to the following dissociation:

$$[001] \rightarrow \tfrac{1}{2}[011] + \tfrac{1}{2}[0\bar{1}1].$$

Only two types of twin were found, α and γ. The thickness of these twins is very variable (from a few hundred ångströms to a few micrometres). The habit planes are always parallel to (100). Fig. 3 shows an α-twin tip: twinning dislocations (Burgers vector $\frac{1}{2}[001]$) can be seen in the matrix–twin interface.

Structural interpretation

When referred to the oxygen sublattice pseudo-cubic cell, the displacement vectors of the stacking faults described above are $\frac{1}{2}[\bar{1}01]_c$ and $\frac{1}{2}[\bar{1}21]_c$; thus the oxygen sublattice is not altered by these faults.

The two types of twins correspond to those that Boland *et al.* (1977) produced by experimental deformation; we will consider them mechanical twins. Our structural interpretation of these twins is based on periodic shear mechanisms for which we will define the planes, vectors and periods as well as their location in the kyanite cell.

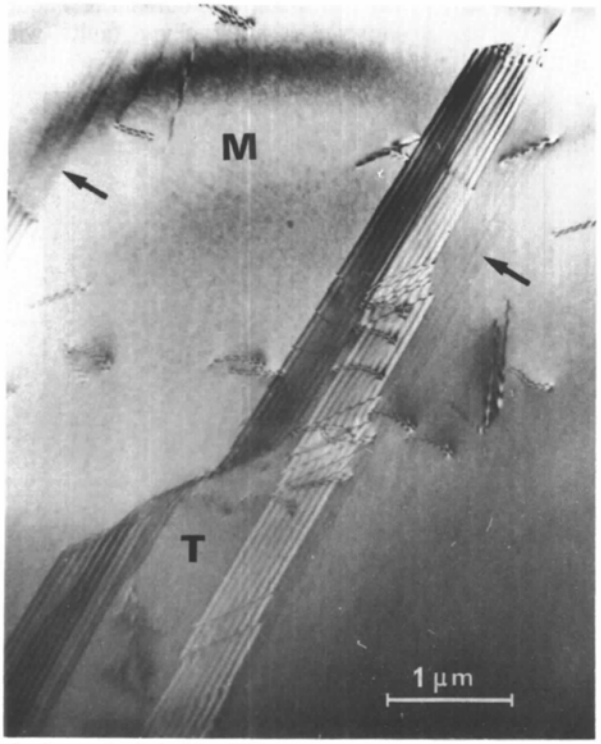

Fig. 3. α-twin tip in Massif Central kyanite. Dark field, $g = 202_M = 30\bar{2}_T$. The $\frac{1}{2}[001]$ stacking faults are out of contrast and arrowed. *M* matrix; *T* twin.

1. *Periodic shears*

(*a*) *Shear plane.* The only dislocation glide system known for kyanite is (100)[001] (Raleigh, 1965; Boland *et al.*, 1977; Ménard, Doukhan & Paquet, 1979) and the matrix–twin interface is always parallel to (100). Thus we selected the (100) plane as shear plane in both cases.

(*b*) *Shear vectors.* The shortest shear vectors suitable for the glide system (100) [001] are $\frac{1}{2}[001]$ and $\frac{1}{2}[011]$. They could correspond to the following dissociations:

$$[001] \rightarrow \tfrac{1}{2}[001] + \tfrac{1}{2}[001]$$

$$[001] \rightarrow \tfrac{1}{2}[011] + \tfrac{1}{2}[0\bar{1}1].$$

These two vectors are also the displacement vectors of the stacking faults described in the previous paragraph.

(*c*) *Shear location.* Fig. 1 is the projection of an idealized kyanite structure on a plane normal to the [001] row; this structure is idealized because it corresponds to the atomic positions given by Náray-Szabó *et al.* (1929) and does not take into account the structure refinement of Burnham (1963). The most likely glide plane for dislocations is shown in Fig. 1: it does not cut the Si–O bonds and does not alter the AlO_6 octahedra chains (Ménard *et al.*, 1977). The layers between these easy glide planes can be considered the most stable structural units in the kyanite structure inasmuch as they are also found in such structures as those of yoderite (Fleet & Megaw, 1962) and staurolite (Náray-Szabó *et al.*, 1929; Griffen & Ribbe, 1973).

(*d*) *Shear period.* This quite naturally follows from what has just been said. It is the distance between easy glide planes, *viz* d_{100}, the reticular distance of the (100) planes.

2. *Mechanical twins*

Fig. 4 shows the α twin resulting from the introduction of the periodic shears $\{(100), \frac{1}{2}[001]\}$ in the kyanite structure: this twin and the matrix are related by a screw diad rotation along [001] (or by a mirror reflection across the plane normal to [001]. It can also be noticed that the twin and the matrix share a complete layer; the corresponding interface must be a low-energy interface, which accounts for the observed habit plane parallel to (100). In the same way, we can obtain the twins corresponding to the $\{(100), \frac{1}{2}[010]\}$ and $\{(100); \frac{1}{2}[011]\}$ periodic shears and demonstrate

that they correspond to the twinning operations shown in Table 2.

Table 2. *Correspondence between periodic shears and twinning operations*

Twinning operations	Periodic shears	
2_1 rotation about [001]	(100), ½ [001]	Observed α twin
2_1 rotation about [010]	(100), ½ [010]	Not observed β twin
b-glide-reflection across (100)	(100), ½ [011]	Observed γ twin

What is remarkable is that these three twins can be produced by periodic shears without additional atomic shuffles as is the case in any other example of mechanical twins in minerals (see, for instance, Biermann, 1980; Kirby & Christie, 1977).

3. *Pseudo-symmetry and layer structure*

The lattice of kyanite is pseudo-orthorhombic. A multiple pseudo-orthorhombic unit cell can be defined by

$$\mathbf{a}_{po} = 4\mathbf{a}_t + \mathbf{b}_t + \mathbf{c}_t$$
$$\mathbf{b}_{po} = \mathbf{b}_t$$
$$\mathbf{c}_{po} = \mathbf{c}_t.$$

The crystalline parameters of these cells are

$a_t = 7{\cdot}119$ Å	$a_{po} = 26{\cdot}82$ Å
$b_t = 7{\cdot}847$	$b_{po} = 7{\cdot}847$
$c_t = 5{\cdot}572$	$c_{po} = 5{\cdot}572$
$\alpha_t = 89{\cdot}98°$	$\alpha_{po} = 89{\cdot}98°$
$\beta_t = 101{\cdot}12$	$\beta_{po} = 89{\cdot}92$
$\gamma_t = 106{\cdot}01$	$\gamma_{po} = 90{\cdot}01.$

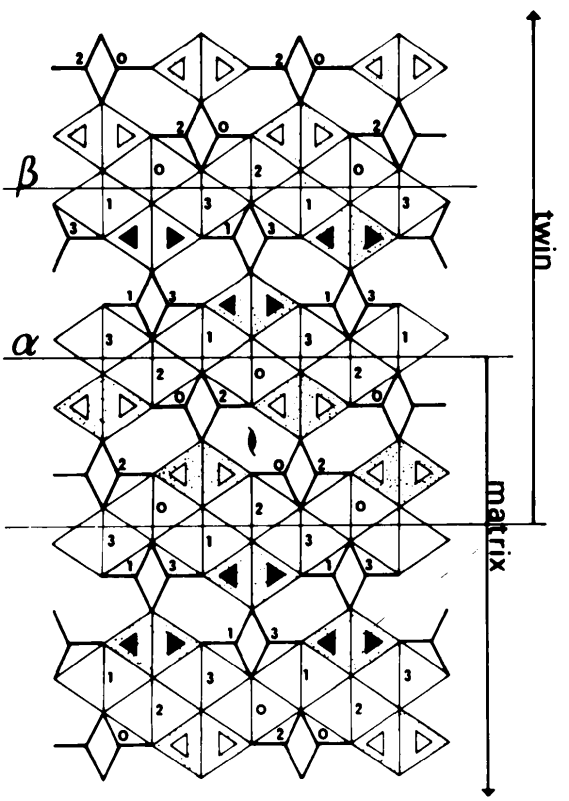

Fig. 4. The upper part is the α twin resulting from the introduction of the periodic shears {(100), ½ [001]} into the kyanite matrix of the lower part. The shear planes are labelled α and β. ⟨ is a screw diad relating the α twin to the matrix.

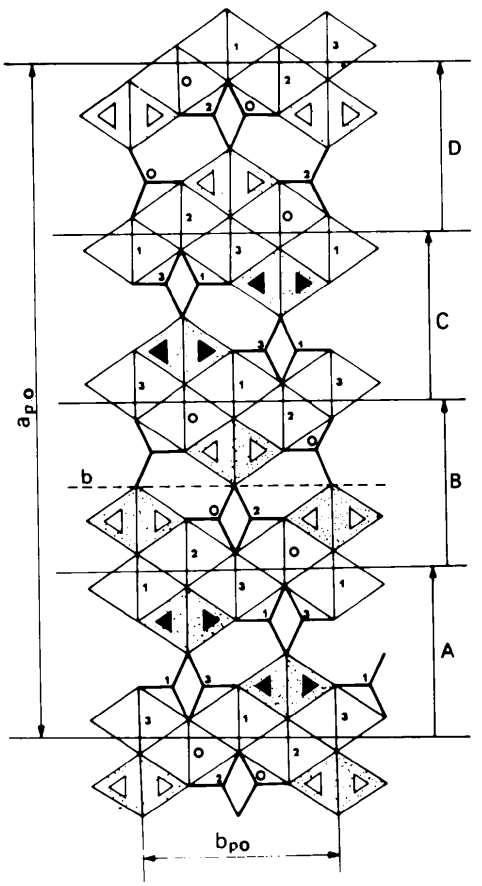

Fig. 5. (001) idealized projection of the pseudo-orthorhombic cell. The stacking sequence involves four layers *A*, *B*, *C* and *D*. The *b*-glide-mirror of the *B* layer is the only one labelled.

Fig. 5 is a (001) projection of this pseudo-orthorhombic cell. It shows that the kyanite structure can be regarded as a periodic stacking of layers *A*, *B*, *C* and *D* (the layers are limited by the glide planes mentioned above). *A*, *B*, *C* and *D* refer to the four possible layer positions in a projection normal to $[100]_{po}$ (going from any layer to its two neighbours requires the vectors $\pm\frac{1}{4}[111]_{po}$). The introduction of the $\frac{1}{2}[011]_t = \frac{1}{2}[011]_{po}$ shear between for instance the *B* and *C* layers turns the

$$\ldots CDABCDAB\ldots$$

stacking into

$$\ldots CDAB/ABCD\ldots.$$

In the unfaulted crystal, the first-neighbouring layers of *B* are *A* and *C*. For the *B* layer that is on the left of the stacking fault, the first-neighbouring layers are *A* and *A*: that is why this fault is thought to be a low-energy one.

Introduction of the periodic shears $\{(100), \frac{1}{2}[011]\}$ on the right of the dotted line turns the stacking

$$\ldots ABCDABC\vdots DABCDAB\ldots$$

into

$$\ldots ABCDABC\vdots BADCBAD\ldots.$$

The latter stacking has a symmetry plane, indicated by the arrowed layer; this plane can only be a symmetry plane relating the two crystals on either side of the dotted line if each layer has its own symmetry plane: this is what Fig. 5 shows. Thus a γ twin has been created. One can also notice that the matrix and the γ twin share a common layer (the arrowed *C* layer in the above example).

Conclusions

The slightly distorted f.c.c. oxygen sublattice of kyanite is not altered by $\frac{1}{2}[001]$ and $\frac{1}{2}[011]$ stacking faults; as much can be said about mechanical twins which have been described by the introduction of these periodic stacking faults in the kyanite matrix.

The structural models proposed for the stacking faults and the twins are based on the fact that the structure of kyanite is of the layered type. Out of the three considered twins leading to low-energy interfaces, only two have been observed (α and γ). We think that the β twins have not been observed because they cannot be mechanically created by **c** dislocations. Experiments are now being conducted to prove this hypothesis.

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