Letter

Hybrid twinning – a cooperative type of oriented crystal association

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Abstract. The reticular theory of twinning is extended to include the contribution of different, coexisting sublattices that consist of quasi-restored nodes (cooperative sublattices) and are characterized by a specific superposition index. The overall degree of quasi-restoration of the twin lattice is a function of the superposition index of the cooperative sublattices, and is expressed by a new parameter, called *effective twin index*, which is the generalization of the classical twin index. Twins where the effective twin index is lower than the classical twin index are termed *hybrid twins*. Several twins (e.g. twins of pyrite and of forsterite) that could not so far be explained by the reticular theory because of their too high twin index are interpreted as hybrid twins. The effect of hybrid twins on diffraction patterns is discussed.

Introduction

An oriented association of natural crystals of the same chemical and crystallographic species in which the individuals are related by an operation not belonging to their vector point group can be called a "twin" at full title if it occurs "frequently" (Hahn and Klapper, 2003). The reticular theory of twinning, as developed by the so-called "French school" (Bravais, 1851; Mallard, 1885; Friedel, 1904, 1926) explains the occurrence probability of twins in terms of overlap of the lattices related by the twin operation: the lower are the twin index and the twin obliquity, the higher is the probability that that twin will form. Friedel (1923) stated that the obliquity plays however a secondary role with respect to the twin index: in other words, a relatively high obliquity is less unfavourable than a relatively high index. This observation, which was often overlooked, is actually rather important in explaining some high-index twins, as we are going to show in this article.

Friedel (1904) introduced as "Mallard's law" the *role of pseudo-symmetry elements as twin elements*[1]. Nowadays, with "Mallard's law" it is often, but improperly, indicated the low probability of occurrence of high-index, high-obliquity twins (see. e.g., Le Page, 2002; Grimmer and Kunze, 2004), where the limit values were set again by Friedel (1904, 1923, 1926) at twin index 6 and obliquity 6°. As a matter of fact, Mallard's analysis of twinned crystals (Mallard, 1885) considered only twins by (pseudo) merohedry: he could not have defined a criterion based on twin index and obliquity, two parameters that were introduced only after Mallard's passing away in 1894 (twin index in Friedel, 1904, p. 218; obliquity in Friedel, 1920). Nevertheless, to refer to Mallard when discussing the occurrence probability of twins in term of their lattice superposition has nowadays become common. Thus, Grimmer and Nespolo (2005), after Th. Hahn (personal communication), suggest rephrasing as "Mallard's criterion" the latter empirical observation, to distinguish it from the original "Mallard's law" established by Friedel and identifying twin elements with direct lattice pseudo-symmetry elements.

For the sake of brevity, in the following we call "Friedelian twins" or "non-Friedelian twins" respectively those twins that obey or violate the criterion of twin index and obliquity not higher than 6 and 6°, respectively. These limits are purely empirical and suffer several exceptions, even at the borderline (ex. the index 7 twin in the Cornish law and Pierre-Levée law of β-quartz twins: Drugman, 1927). Some crystal associations with much higher index have been described as *plesiotwins* (Nespolo et al., 1999b). In these latter associations, the coalescence of

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[1] "Les plans et axes d'ordre *n* de pseudo-symétrie du réseau simple (plans réticulaires et rangées) peuvent jouer le rôle de plans de macle et d'axes de macle d'ordre *n*" (Friedel, 1904, p. 157). Later formulation: "Quand le réseau-période a des plans ou des axes de pseudo-symétrie, ces plans (réticulaires) et axes (rangées) peuvent être plans et axes de macle" (Friedel, 1926, p. 436).

Table 1. Some mineralogical examples of non-Friedelian twins, and their interpretation as hybrid twins when possible. Twin laws after Palache et al. (1952). The cell parameters used in the computation of twin index and obliquity are taken from the Mineralogy Database (http://webmineral.com/).

Compound	Space-group type	First component (index/obliquity)	Second component (index/obliquity)	Third component (index/obliquity)	Hybrid twin	Effective twin index
Pyrite FeS_2	$Pa\bar{3}$	(052)/[052] (29/0°)	(052)/[021] (6/5.5°)	(021)/[052] (6/5.5°)	yes	3.2
Galena PbS	$Fm\bar{3}m$	(025)/[025] (29/0°)	(025)/[012] (12/4.8°)	(012)/[025] (12/4.8°)	yes	5.8
Forsterite Mg_2SiO_4	*Pbnm*	(012)/[016] (13/0.5°)	(012)/[029] (10/4.4°)	(023)/[016] (10/5.5°)	yes	4.3
Euxenite-(Y) $(Y,Ca,Ce)(Nb,Ta,Ti)_2O_6$	*Pcan*	(201)/[704] (9/0°)	(201)/[201] (5/3.0)	–	yes	3.6
Enargite Cu_3AsS_4	$Pnm2_1$	(201)/[704] (9/0°)	(201)/[201] (5/3.0°)	–	yes	3.6
Tantalite $FeTa_2O_6$	*Pcan*	(201)/[11 0 7] (29/0°)	(201)/[201] (5/5.5°)	–	yes	4.8
Chalcostibite $CuSbS_2$	*Pnam*	(104) [1 0 10] (41/0°)	(104)/[001] (2/9°)	(001)/[1 0 10] (5/9°)	yes	1.4
Maucherite $Ni_{11}As_8$	$P4_{1,3}2_12$	(106)/[302] (15/2.6°)	(106)/[201] (4/4.3°)	(105)/[302] (13/7.1°)	yes	3.0
		(203)/[13 0 2] (16/0.7°)	(203)/[5 0 1] (13/7.1°)	–	yes	8.0
Galena PbS	$Fm\bar{3}m$	(114)/[114] (9/0°)			no	–
Pyrargyrite Ag_3SbS_3	$R3c$	(104)/[2 0 13] (27/0.1°)	–	–	no	–
Staurolite $(Fe,Mg)_2Al_9(Si,Al)_4O_{20}\,(O,OH)_4$	$C2/m$ ($\beta = 90°$)	(231)/[313] (12/1.3°)	–	–	no	–

post-grown crystals and the surface effect are supposed to play an important role, so that their formation mechanism is different from those typical of growth twins (Nespolo and Ferraris, 2004a). Nevertheless, real non-Friedelian twins do exist and are known since long ago; for example they are not rare in some common minerals studied in details mainly on the basis of their morphology (see Table 1). For these high-index twins the classical reticular explanation is hardly satisfying and needs to be somehow extended to include the contribution of different but closely related sublattices. Non-Friedelian twins where this phenomenon is observed are here defined *hybrid twins*.

Twins law, twin index and twin obliquity

Pairs of individuals in a twin are related by a twin operation. In general, more than one such operation may exist; when the common symmetry of the individuals (intersection group of the oriented point groups) is higher than 1, these operations are either equivalent or quasi-equivalent under the action of the symmetry elements of the individual. A set of (quasi) equivalent twin operations forms a *twin law*; this set of operations constitutes a coset of the twin point group with respect to the individual point group (Hahn and Klapper, 2003). A twin operation is performed about a twin element, which is a symmetry element for the twin lattice but not for the individual crystal. The twin lattice, $\mathbf{L}_T$, either coincides with the individual lattice, $\mathbf{L}_I$, or is a sublattice of it. The cell of the twin lattice is defined (i) by the period of the row corresponding to the twin axis [*uvw*] and by the conventional mesh of the net (*hkl*) that is (quasi) normal to it; or (ii) by the conventional mesh of the net corresponding to the twin plane (*hkl*) and by the period of the lattice row [*uvw*] that is (quasi) normal to it. The ratio of the volumes of the cells of $\mathbf{L}_T$ and $\mathbf{L}_I$, scaled by the their multiplicities, is the twin index mentioned above. It corresponds to the ratio of the number of lattice nodes in the cell of the $\mathbf{L}_T$ to the number of lattice nodes restored by the twin operation. From the indices of the twin element – [*uvw*] or (*hkl*) – the twin index can be obtained as follows (Friedel, 1926; Donnay and Donnay, 1959). Given $S = |hv + kw + lw|$, the twin index n can take the values S, $S/2$, $S/4$ depending on the type of centring of $\mathbf{L}_I$, and on the parities of h, k, l, u, v, w and S (Table 2). When $\mathbf{L}_T$ coincides with $\mathbf{L}_I$, the twin index is 1.

The coincidence between $\mathbf{L}_T$ and $\mathbf{L}_I$, or a sublattice of the latter, may be approximate. Because a lattice is always holohedral, to a (pseudo) mirror plane always corresponds a (pseudo) symmetry axis (quasi) normal to it, and vice versa. The obliquity ω can be defined either as the angle between the lattice plane quasi normal to the twin axis and the plane (in general not rational in the direct space) perpendicular to it (rotation twins); or as the angle between the lattice row quasi perpendicular to the twin plane and the direction (in general not rational in the direct space) perpendicular to it (reflection twins). All twins of cubic crystals have zero obliquity: in fact, in a cubic crystal the lattice row [*hkl*] and the lattice plane (*hkl*) are mutually perpendicular.

This classification in terms of twin index and obliquity leads to the well-known four classical categories of twins by [reticular] (pseudo) merohedry (Friedel, 1926).

A finer classification has been recently introduced (Nespolo and Ferraris, 2000, 2004b) to take into account

Table 2. Computation of the twin index as a function of $S = |hv + kv + lw|$ and of the lattice centring (see Friedel, 1926; Donnay and Donnay, 1959).

Lattice centring	Condition on h, k, l	Condition on u, v, w	Condition on S	n
P	none	None	S odd	$n = S$
			S even	$n = S/2$
C	$h + k$ odd	None	none	$n = S$
	$h + k$ even	$u + v$ and w not both even	S odd	$n = S$
			S even	$n = S/2$
		$u + v$ and w both even	$S/2$ odd	$n = S/2$
			$S/2$ even	$n = S/4$
B	$h + l$ odd	None	none	$n = S$
	$h + l$ even	$u + w$ and v not both even	S odd	$n = S$
			S even	$n = S/2$
		$u + w$ and v both even	$S/2$ odd	$n = S/2$
			$S/2$ even	$n = S/4$
A	$k + l$ odd	None	none	$n = S$
	$k + l$ even	$v + w$ and u not both even	S odd	$n = S$
			S even	$n = S/2$
		$v + w$ and u both even	$S/2$ odd	$n = S/2$
			$S/2$ even	$n = S/4$
I	$h + k + l$ odd	None	none	$n = S$
	$h + k + l$ even	u, v, w not all odd	S odd	$n = S$
			S even	$n = S/2$
		u, v, w all odd	$S/2$ odd	$n = S/2$
			$S/4$ even	$n = S/4$
F	none	$u + v + w$ odd	none	$n = S$
	h, k, l not all odd	$u + v + w$ even	S odd	$n = S$
			S even	$n = S/2$
	h, k, l all odd	$u + v + w$ even	$S/2$ odd	$n = S/2$
			$S/4$ even	$n = S/4$

special cases of merohedry (syngonic merohedry, metric merohedry) and the point isosymmetry of lattice vs. sublattice differently oriented (reticular polyholohedry). Recent reviews on twins can be found in Hahn and Klapper (2003) and Ferraris et al. (2004); a critical analysis of the use of the concept of "twinning" as structure-building and crystal-association mechanism is presented by Nespolo et al. (2004).

Hybrid twins and effective twin index

Several non-Friedelian twins – reported more than once, and thus not just occasional associations – are known that correspond to a surprisingly high twin index (some examples are given in Table 1). The determination of the twin element was obtained either by morphological studies – it is the case of old mineralogical examples – or by diffraction methods. Some of these unusual twins can actually be explained by extending the classical reticular theory of twins.

Let (*hkl*) and [*uvw*] be a pair of mutually (quasi) perpendicular (pseudo) symmetry elements for the lattice of the individual, or a sublattice of it. When one of these elements is not a symmetry element for the motif, it may act as twin element (twin plane, twin axis). When neither of them is a symmetry element for the motif, both can act as twin elements: if the perpendicularity is only approximate, the result is a pair of twins that are non-equivalent even in centrosymmetric crystals: they are known as *corresponding twins* (Friedel, 1926).

The pair (*hkl*)/[*uvw*] defines the cell of the twin lattice, $\mathbf{L}_T$, the twin index n and the twin obliquity ω. The corresponding twin operation restores one node out of n of $\mathbf{L}_I$, and the Bravais cell of $\mathbf{L}_T$ is defined by these restored nodes. The other $n - 1$ nodes are not restored: this means that corresponding vectors from the origin in the lattices $\mathbf{L}_i$ and $\mathbf{L}_j$ are separated by an angle φ. The minimal value of this angular separation decreases however with the increase of the twin index and for relatively high values of n it may happen that a second subset of lattice nodes is *approximately* restored. When this second subset consists of a fraction of lattice nodes significantly higher than $1/n$ and the corresponding angular separation φ is small (namely close to the Friedelian limit for the obliquity), it should be reasonably taken into account as concurrent with the first subset in establishing Friedelian conditions of twinning. This second subset of nodes defines another sublattice $\mathbf{L}_A$, based on a smaller cell; for reflection twins this sublattice is based on the same twin plane (*hkl*) but on an alternative lattice row $[u_A v_A w_A]$; for rotation twins it is instead based on the same twin axis [*uvw*] and on an alternative lattice plane $(h_A k_A l_A)$. The cell of $\mathbf{L}_A$ defines a *superposition index*, n_A, smaller than the twin index n, and an obliquity ω_A, related to φ, that is non-zero but still within the Friedelian limits. The result is a hybrid between reticular merohedry and reticular pseudo-merohedry, and for this reason it is here defined as *hybrid twin*. When the original twin law corresponds to a non-zero obliquity ω, the hybrid twin consists of two reticular pseudo-merohedries.

By extending the above arguments, one could foresee cases in which N sublattices contribute to the hybrid twin. Let the first sublattice be the one with minimal obliquity ($\omega_{\min} = \omega_1$) but high index n_1 and the N-th sublattice the one with minimal index $n_N = n_{\min}$, but high obliquity; the other sublattices have intermediate values of both the index and the obliquity:

$$n_1 > n_2 > n_3 > \ldots > n_N ,$$

$$\omega_1 < \omega_2 < \omega_3 < \ldots < \omega_N .$$

However, for $n_2, n_3 \ldots n_{N-1}$ to be within Friedelian limits n_1 should be rather high and n_N fairly low: these two conditions are contradictory, because in such a case the twin would be Friedelian, with twin index n_N. As a consequence, in the analysis of a hybrid twin we consider the twin as deriving from the coexistence of up to three sublattices: 1) the lowest-obliquity sublattice — the limit on the twin index being significantly relaxed with respect to the Friedelian limit; 2) the lowest-index non-zero obliquity sublattice based on the lowest-obliquity twin plane; and 3) the lowest-index non-zero obliquity sublattice based on the lowest-obliquity twin axis. The cells of the three lattices are described as follows:

1. $(hkl)/[uvw]$, $\omega \geq 0$, n
2. $(hkl)/[u_A v_A w_A]$, $\omega_A > \omega$, $n_A < n$
3. $(h_B k_B l_B)/[uvw]$, $\omega_B > \omega$, $n_B < n$.

In cubic crystals $\omega = 0$, $u_A = h_B$, $v_A = k_B$ and $w_A = l_B$ and thus $\omega_A = \omega_B > 0$ and $n_A = n_B$.

When in a non-Friedelian twin at least one between n_A and n_B is close to the Friedelian limit, the fraction of nodes of $\mathbf{L}_I$ that is restored within the Friedelian limit on the obliquity is a function of up to three twin indices: n, n_A and n_B. In fact, if $\mathbf{L}_T$ is the twin lattice defined, as usual, by the nodes belonging to the $(hkl)/[uvw]$ cell, $\mathbf{L}_A$ and $\mathbf{L}_B$ are the corresponding lattices defined by the nodes of the $(hkl)/[u_A v_A w_A]$ and $(h_B k_B l_B)/[uvw]$ cells respectively: $1/n$, $1/n_A$ and $1/n_B$ are the fractions of nodes restored by the twin operation within the limits of the obliquities ω, ω_A and ω_B respectively. The total number of nodes quasi-restored in the cell of $\mathbf{L}_T$ is thus a function of the number of nodes of $\mathbf{L}_A$ and $\mathbf{L}_B$ contained in the cell of $\mathbf{L}_T$. The cell of $\mathbf{L}_T$ contains $S_T = S/n$ nodes of $\mathbf{L}_T$, $S_A = \mathrm{int}\,(S/n_A)$ nodes of $\mathbf{L}_A$ and $S_B = \mathrm{int}\,(S/n_B)$ nodes of $\mathbf{L}_B$, where "int (x)" is the integer part of x. We now introduce a new index $n_E = S/(S_T + S_A + S_B)$ which, in general, is no longer integer, and call it *effective twin index*. For a Friedelian twin, n_E reduces to the classical (integer) twin index n, in the same way the *effective coordination number* reduces to the classical, integer coordination number for regular polyhedra (Hoppe, 1979).

The introduction of the concept of hybrid twins permits to rationalize some of the twins that were so far considered non-Friedelian (Table 1). Hereafter we present the detailed analysis of two cases.

Case study 1: the {052} twin in pyrite

Although the most frequent twin in pyrite (space group $Pa\bar{3}$, $a = 5.417$ Å) is the common spinel law $\{111\}/\langle 111\rangle$, twin index 3, several other twins have been reported too, some of which (Smolař, 1913) are definitely non-Friedelian. Among these, a non-negligible number of twins have been found repeatedly, excluding thus the possibility of an accidental association. Here we take the {052} twin as a first case study of hybrid twin, because of its high twin index, and because the cubic symmetry of the individual makes particularly simple the analysis and graphical interpretation. For the calculation of the twin index see Table 2; the obliquity is obtained as the angle between $[uvw]$, the rational direction quasi-normal to (hkl), and $[hkl]^*$, the reciprocal-lattice direction normal to (hkl).

In a cubic crystal, each (hkl) plane is perpendicular to the $[hkl]$ direction. Therefore, the cell of $\mathbf{L}_T$ is in our case defined by (052)/[052], which results in the twin index $n = 29$. Such a high index puts the twin outside the possibility of interpretation on the basis of the classical reticular theory, despite the zero obliquity; i.e., it is clearly a non-Friedelian twin. Nevertheless, among the 28 nodes out of 29 that are not restored by the twin operation, some are quasi-restored and their contribution should not be ignored in the reticular interpretation of this twin.

Fig. 1a shows the (100) plane of $\mathbf{L}_I$ and the corresponding projection of the cell based on the (052)/[052] pair; $[02\bar{5}]$ is the direction representing the trace of the (052) plane on (100). Lattice nodes are represented by "0", the nodes not restored by the twin operation, and "4", the nodes restored by the twin operation. The latter nodes thus correspond to the corners of the twin lattice cell built on (052)/[052].

The direction [021] makes with the twin axis [052] an angle of 4.76°, which is within the limits of a Friedelian obliquity. We can therefore define an alternative cell, $\mathbf{L}_A$, based on (052)/[021], for which the superposition index is 6 (Fig. 1b). The mesh of $\mathbf{L}_A$ in the (100) plane is centred: not only nodes at its corners, but also those centring the cell (nodes $02\bar{2}$ and 003 in the axial setting of the individual) are quasi-restored by the twin operation; they are indicated as "1". All the other nodes are indicated as "0". Exactly in the same way, the plane (021) makes an angle of 4.76° with (052), and thus we can define a further alternative cell, $\mathbf{L}_B$, based on (021)/[052] for which the superposition index is again 6 (Fig. 1c): $[01\bar{2}]$ is the direction representing the trace of the (021) plane on (100). The mesh of $\mathbf{L}_B$ in the (100) plane is centred: not only nodes at its corners, but also those centring the cell (nodes 022 and $00\bar{3}$ in the axial setting of the individual) are quasi-restored by the twin operation; they are indicated as "2". All the other nodes are indicated as "0".

Finally, Fig. 1d is the superposition of Fig. 1a, 1b and 1c. The numerical value in correspondence of each node is the sum of the values in the three figures and permits to identify without ambiguities the components. The node at the origin is indicated as "7", because it is common to the three cells, $\mathbf{L}_T$, $\mathbf{L}_A$ and $\mathbf{L}_B$ ("1" + "2" + "4"). Nodes indicated as "6" are common to the cells of $\mathbf{L}_T$ and $\mathbf{L}_B$ ("4" + "2"). Nodes indicated as "5" are common to the cells of $\mathbf{L}_T$ and $\mathbf{L}_A$ ("4" + "1"). Nodes indicated as "3" are

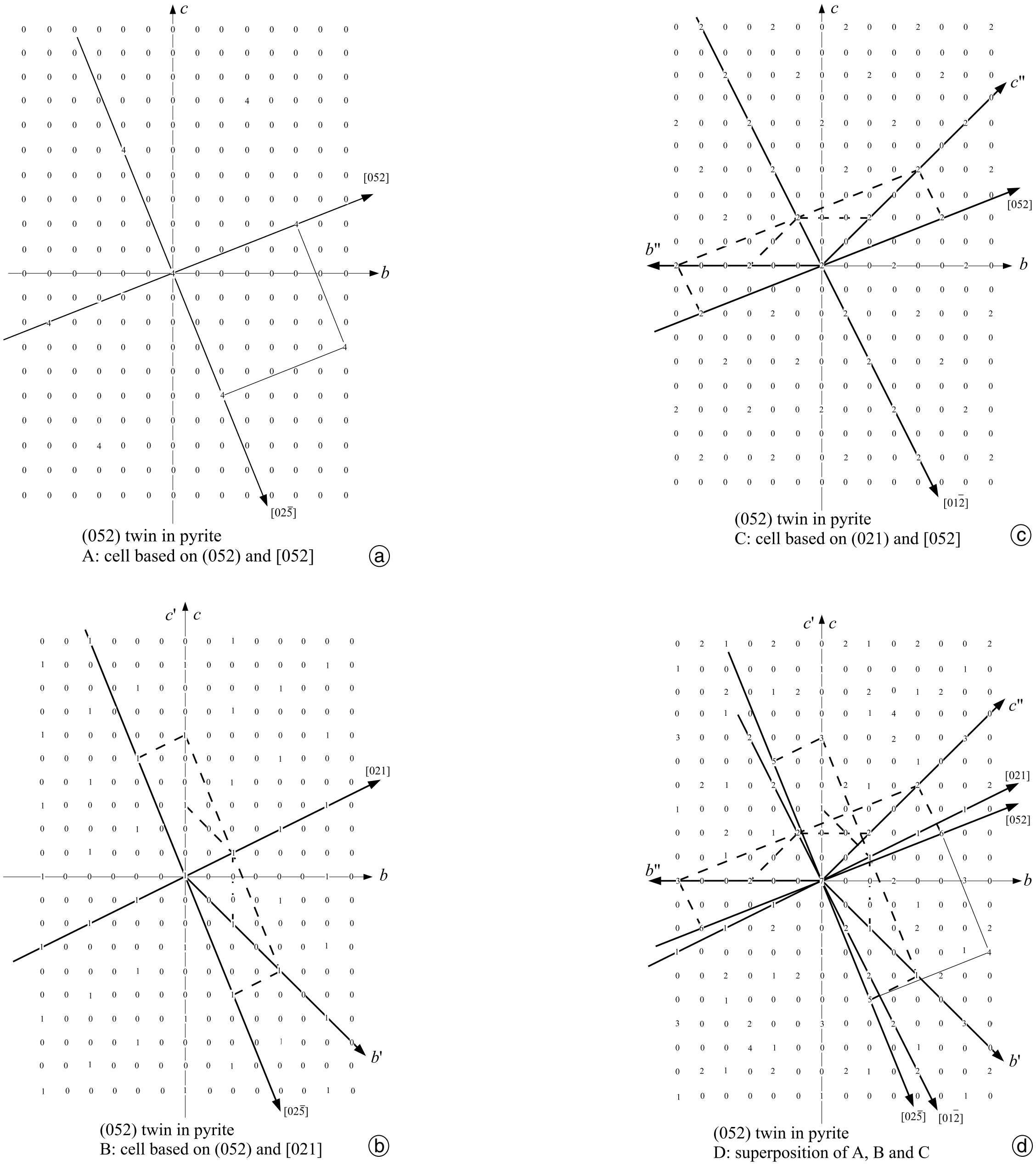


Fig. 1. Interpretation of the (052) twin in pyrite as hybrid twin. (**a**) (100) plane of the lattice of the individual, with the twin-lattice cell defined by the pair (052)/[052]: twinning by reticular merohedry, index 29, obliquity zero. Nodes restored exactly by the twin operations are shown as "4", those not restored as "0". (**b**) A smaller cell (cell of $\mathbf{L}_A$) is defined by the pair (052)/[021], which corresponds to a subset of nodes of $\mathbf{L}_I$ (superposition index 6) quasi-restored (obliquity 4.76°) by the twin operation ("1"). $[02\bar{5}]$ is the direction representing the trace of the (052) plane on (100). The cell of $\mathbf{L}_A$ is A centred and a-unique monoclinic and can be transformed into an mP cell defined by the transformation $cP \to mP$ $(100/02\bar{2}/003)$ (matrix read by columns). The axes of the mP cell are indicated as b' and c'. (**c**) The cell of $\mathbf{L}_B$ is defined by the pair (021)/[052], which corresponds to a second subset of nodes of $\mathbf{L}_I$ quasi-restored (same superposition index and obliquity as $\mathbf{L}_A$) by the twin operation ("2"). $[01\bar{2}]$ is the direction representing the trace of the (021) plane on (100). As in the case of $\mathbf{L}_A$, the cell of $\mathbf{L}_B$ is A centred and a-unique monoclinic, and is the transformed into an mP cell by the matrix transformation $cP \to mP$: $(\bar{1}00/0\bar{3}0/022)$. The axes of the mP cell are indicated as b'' and c''. (**d**) Hybrid twin obtained by overlapping (a), (b) and (c). The numeric code assigned to each node shows whether a node is (quasi)restored by any of the three pairs (non-zero code) or not (zero code). The numerical value of the codes is the sum of the corresponding values in each of the three pairs, and the result identifies uniquely the pairs (quasi)restoring the corresponding node.

common to the cells of $\mathbf{L}_A$ and $\mathbf{L}_B$ ("2" + "1"). Nodes indicated as "1", "2" and "4" belong to one cell only.

The cell of $\mathbf{L}_T$ contains $S_T = 1$ node of $\mathbf{L}_T$, $S_A = \text{int}(29/6) = 4$ nodes of $\mathbf{L}_A$ and $S_B = \text{int}(29/6) = 4$ nodes of $\mathbf{L}_B$, and the effective twin index is $n_E = S_E = 29/(1+4+4) = 3.2$ (Fig. 1d).

The twin under consideration, rather than a non-Friedelian twin by reticular merohedry with index 29, is a hybrid twin that, on reticular basis, is cooperatively supported by three different sublattices implying both reticular merohedry and reticular pseudo-merohedry; its effective twin index is 3.2 and has a composite obliquity (0, 4.76). Obviously, non-zero obliquity twin laws in cubic crystals are meaningful only as components of hybrid twins, when the zero-obliquity law corresponds to a high-index non-Friedelian twin.

Finally, it must be pointed out that the pair (021)/[021] cannot represent the twin law for the observed twin. In fact, the measured morphological angle is 43°36′, which corresponds to (052) as twin plane, whereas (021) as twin plane requires 53°8′ and corresponds to another, different twin.

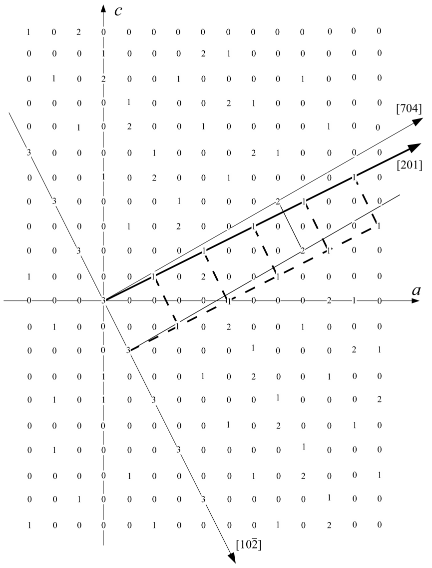
To be noted that the same type of analysis here proposed for the {052} twin of pyrite applies to all cubic crystals showing the same twin law because in the cubic system the twin laws do not depend on the cell parameter. However, the effective twin index is affected by the Bravais type of $\mathbf{L}_\mathrm{I}$. The same twin has been reported in galena, which however has a *cF* lattice type, instead of *cP* as in the case of pyrite. Therefore, $n_\mathrm{A} = n_\mathrm{B} = 12$, $S_\mathrm{A} = S_\mathrm{B} = \mathrm{int}\,(29/12) = 2$, $n_\mathrm{E} = 29/(1 + 2 + 2) = 5.8$ (Table 1).

Case study 2: euxenite and enargite {201} twins

Euxenite-Y (Y,Ca,Ce)(Nb,Ta,Ti)$_2$O$_6$ (*Pcan*, $a = 5.52$, $b = 14.57$, c = 5.166 Å) and enargite Cu$_3$AsS$_4$ (*Pnm*2$_1$, $a = 6.41$, $b = 7.42$, $c = 6.15$ Å) give a twin with twin plane (201). The *c*/*a* ratio close to 0.95 makes the direction normal to (201) a rational direction with relatively low indices, [704]. The cell of $\mathbf{L}_\mathrm{T}$ is *mB*, the twin is index 9 and the obliquity zero. Not far from [704] another lattice direction, [201], has a shorter periodicity and defines a smaller cell of type *mP*: the pair (201)/[201] defines the $\mathbf{L}_\mathrm{A}$ sublattice which corresponds to a superposition index of 5 and an obliquity of 3.0°.

Fig. 2 shows the cells of $\mathbf{L}_\mathrm{T}$ (nodes "2"), of $\mathbf{L}_\mathrm{A}$ (nodes "1"), and common to both cells (nodes "3"). Because $S_\mathrm{T} = 2$ and $S_\mathrm{A} = \mathrm{int}\,(18/5) = 3$, the effective twin index is $n_\mathrm{E} = \mathrm{S}_\mathrm{E} = 18/(2 + 3) = 3.6$. Twinning in this example is a hybrid between a reticular merohedry and a reticular pseudo-merohedry.

Whereas one might simply describe this twin as a twin by reticular pseudo-merohedry, because both the index and the obliquity are within the Friedelian limits, the cell based on (201)/[704] cannot be ignored: despite the relatively high (but not prohibitive) twin index, the zero obliquity makes the contribution from this pair not negligible. It would be in fact hardly justifiable to accept as correct description of the twin the overlap of one node out of five approximated by 3° and to reject the *exact* overlap to one node out of nine. This example shows thus that some Friedelian twins close to the limits of Mallard's criterion may actually be better considered hybrid twins, at least under specific metric conditions. The criterion to judge the significance of the contribution from a second (third) pair is the value of the effective twin index with respect to the classical twin index corresponding to the Friedelian twin.



(021) twin in euxinite-Y and in enargite

Fig. 2. Reticular interpretation of the {201} twin in euxenite-(Y) and enargite. [704] is the direction perpendicular to the twin plane. [10$\bar{2}$] is the direction representing the trace of the (201) plane on (010). Nodes exactly restored by the twin operation define the cell of $\mathbf{L}_\mathrm{T}$, based on the pair (201)/[704] and are shown as "2". (201)/[201] is an alternative pair based on quasi-restored nodes ("1") defining the smaller cell $\mathbf{L}_\mathrm{A}$. Nodes common to both cells are indicated as "3".

Discussion

Following Friedel, the occurrence of a twin has been here discussed in terms of the lattice; nevertheless, this occurrence also depends on the atomic coherence at the composition surface, which may be two-dimensional, in case of contact twins, or extended within the bulk of the individuals, for penetration twins (see, e.g., Buerger, 1945; Holser, 1958). To describe the degree of *atomic* overlap produced by the twin operation, Takeda et al. (1967) introduced the concept of *restoration index*, which is the structural counterpart of the twin index.

The two approaches are not in contradiction. In fact, the structural motif in a crystal is repeated with the periodicity of the lattice, a high degree of coincidence of the lattices of the individuals corresponds to a high degree of continuity of the structural motif in the different, non-equivalent orientations of the individuals. On this basis, the reticular theory of twinning was able to explain the occurrence and formation probability of most twins, and is still useful for extensions (see Nespolo et al., 1999a, b, c; Nespolo and Ferraris, 2000). In particular, the so-called "Mallard's criterion" ranks the probability of occurrence of a twin on the basis of its twin index and obliquity. Twins that do not satisfy this criterion (here called non-Friedelian twins) should occur only exceptionally and probably in conditions far from the thermodynamic equilibrium. Actually, they are rarer than the low-index twins, but not so rare to be considered exceptions to a criterion or occasional associations formed under unique conditions.

We have shown that in several cases the occurrence of non-Friedelian twins can still be explained on the basis of the classical reticular theory by introducing the concepts of hybrid twin and effective twin index. The Mallard's criterion on the twin index and twin obliquity has been essentially retained, but applied to the whole hybrid twin.

A non-Friedelian twin corresponds to a hybrid twin when its high twin index implies the near-superposition of at least a second sublattice with higher degree of quasi-restoration. In this respect, Friedel's statement that the twin obliquity plays a secondary role in determining the probability of occurrence of a twin has to be read under a new light. In fact, the second sublattice corresponds to a higher obliquity but also to a higher degree of superposition, and its contribution to the global restoration of lattice nodes is essential to explain the occurrence of such twins.

It should also be emphasized that the importance of a relatively high degree of quasi-restoration, when the degree of exact restoration is too low to be considered meaningful, was already pointed out by Sueno et al. (1971), with the introduction of the concept of *pseudo-tessellation*. It was however employed in the special case of two-dimensional regular aggregates of layered crystals, which are more directly connected to plesiotwins than to hybrid twins. Its role in twins was instead not realized before.

Some examples of non-Friedelian twins that cannot be explained as hybrid twins remain, one of which is the common 60° twin in staurolite, twin index 12, which does not satisfy the conditions here established for a hybrid twin (see Table 1). This shows that the Friedelian lattice conditions, even with the extension introduced by this paper, may not be sufficient to explain all known twins. The application of the concept of *lattice complex* (see, e.g., Fischer et al., 1973) to twinning has sometimes given a structural support to the reticular explanation, as in the case of pyrite and digenite analysed by Donnay and Curien (1960); a subset of the atoms occupy the Wyckoff positions corresponding to a lattice complex and are common to the whole twinned edifice, whereas the others have different orientation in each individual. It is possible that the same argument may help explaining the occurrence of non-Friedelian non-hybrid twins, although to date we are not aware of any example.

Another possible explanation comes from the study of the atacamite twins, which have been interpreted in terms of parallelism of atomic chain-links, instead of lattice rows (Hartmann, 1960).

The character of hybrid twin may be revealed by a careful analysis of the diffraction pattern. When the hybrid twin consists of pseudo-reticular merohedries, a few reflections are almost superposed (split reflections): they correspond to the $\mathbf{L}_\mathrm{T}$ lattice, which is characterized by a large twin index n, i.e. a small fraction $1/n$ of quasi-restored nodes. A larger number of reflections are not superposed but separated by a small angle φ: they correspond to the $\mathbf{L}_\mathrm{A}$ ($\mathbf{L}_\mathrm{B}$) lattices ($1/n_\mathrm{A}$ and $1/n_\mathrm{B}$ are larger than $1/n$). The rest of the diffraction pattern is composed of reflections that are farer apart: they correspond to the part of $\mathbf{L}_\mathrm{I}$ that does not contribute to the above sublattices.

When the hybrid consists of a reticular merohedry and one (two) reticular pseudo-merohedry, the situation is the same but the reflections corresponding to $\mathbf{L}_\mathrm{T}$ are exactly superposed.

On the whole, the appearance of the diffraction pattern of a hybrid twin is the same as in a reticular pseudo-merohedry. The few superposed reflections, if not recognized as such, will however reduce the quality of the refinement; their recognition requires however a full understanding of the twin law.

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