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CLASSIFICATION OF TRIPERIODIC TWINS

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The classification of twins based on the theory that was elaborated by the French crystallographers from Bravais and Mallard to Friedel (1904; Internat. Tables 1959) dates back, of course, to pre-x-ray days, when twins could only be studied morphologically by means of goniometry (contact and reflection goniometers). Nowadays, when we suspect a specimen to be twinned we must still examine in detail any available morphological evidence of twinning, but we then proceed to the x-ray studies, in particular "precession goniometry" (Donnay *et al.* 1955; Donnay & Donnay 1967; Chen & Chao 1973), where we examine precession orientation and cone-axis photographs for twin information. What do we observe?

The patterns will show either a single orientation of the reciprocal lattice or two (or more) distinct orientations having a common origin. In the first case, there will be no obvious evidence of twinning, such as doubling of spots, and it may take a high, irreducible residual R in the attempted crystal-structure determination to indicate the presence of twinning. (For an illustration see, for example, the case of harmotome, Hoffman *et al.* 1973). If twinning is indeed present, this case will be called: *twinning by twin-lattice symmetry*, TLS. The alternate case, when more than one orientation of the reciprocal lattice is observed, becomes *twinning by twin-lattice quasi-symmetry*, TLQS. These two groups represent the primary division of the twin kingdom because they are instantly distinguishable on orientation precession films.

The further subdivision rests on the concept of twin index, n, defined as follows:

n = (vol. per node in twin lattice)/(vol. per node in crystal lattice). The twin lattice is the lattice with the smallest cell that is common to both individuals of the twin. At the composition surface it will show perfect continuity for the case of TLS, but will suffer a slight deviation for TLQS specimens. For $n = 1$, the twin lattice coincides with the crystal lattice; for $n > 1$, the twin lattice is a superlattice† of the crystal lattice in direct space and a sublattice in reciprocal space.

A sample with TLS and n equal to unity is the most difficult to recognize by x-ray diffraction alone, as mentioned above. Several specimens may have to be measured and their corresponding $F(hkl)$ values compared, in order to rule out this type of twinning, and even then the investigator may be fooled, because the relative volume proportions of the various individuals in the twin may be constant, thus leading to comparable but not true $F(hkl)$ values. The common twins of quartz (Table 1) illustrate the point; the accepted structure determination by Young & Post (1962) of low-temperature quartz must have been based on twin data (R. F. Stewart, priv. com.).

A twin by TLS with $n>1$ usually has $n=3$ and almost always shows peculiar "systematic" absences that are neither space-group nor structural ones and may well be called "twin absences". Their presence, when identified as such, permits recognition of twinning by TLS with $n = 3$.

For the case of TLQS, the twin law, in reciprocal space, is usually readily established on x-ray precession patterns from the lattices of the individual component crystals. The determination of the twin index, which may have any integral value but is usually below six, is readily accomplished. Table 1 summarizes the proposed classification and gives at least one well-known example for each of the four categories.

In conclusion it may be pointed out that Niggli (1919, 1920, 1941) had already rearranged

† Geometrically the twin lattice could equally well be a sublattice in direct space, as pointed out by Friedel (1904, 1926). Wrinch (1952) was the first to switch from the superlattice to the sublattice — the only one that has a crystal-structure significance and led to the concept of "index of restoration" (Takeda *et al.* 1967).

TABLE 1. CLASSIFICATION OF TWINS

Twinning by:	Twin-lattice symmetry (TLS)		Twin-lattice quasi-symmetry (TLQS)	
Twin obliquity ω	$\omega = 0$ (rigorously)		$\omega > 0$, ω always small, may be ~0, rarely >5°	
Composition surface	usually irregular (penetration twins), can be planar though need not be		planar and parallel to twin plane (contact twins), or parallel to twin axis; planar "rhombic section"† if 2-fold twin axis; not necessarily planar if m-fold twin axis, m>2.	
Twin lattice	crystal lattice	super- or sub-lattice	crystal lattice	super- or sub-lattice
Twin index n	$n = 1$	n = 3 or (rarely) 5††	$n = 1$	$1 < n < 6$
Examples	low quartz	calcite	plagioclases	clinopyroxene
Twin name (twin "law")	Dauphiné;Brazil	Basal twinning	Albite; Pericline	...
Crystal point group	32	$\bar{3}\ 2/m$	$\bar{1}$	$2/m$
Twin operation(s)	$[0001]_{180°}$; $(11\bar{2}0)$ *etc.* *etc.* all the operations of the next higher merohedry	(0001), *etc.*	(010);$[010]_{180°}$	(100)
Twin symmetry§	$6'22'$; $\bar{3}''2/m''$	$\frac{6'}{m'}\frac{2}{m}\frac{2'}{m'}$	$\frac{2^{*\prime}}{m'}$; $\frac{2''}{m^{*\prime\prime}}$	$\frac{2^{*\prime}}{m'}\frac{2}{m}\frac{2'}{m^{*\prime}}$
Complete twin symmetry	$\frac{6'}{m'''}\frac{2}{m''}\frac{2'}{m'''}$ $(\bar{1}'')$		$\frac{2''}{m'}$ $\bar{1}$	
Friedel's nomenclature (1904)	by merohedry	by reticular merohedry	by pseudo-merohedry	by reticular pseudo-merohedry
Niggli's nomenclature (1919, 1920, 1941)	Meroedrische Zwillinge s.v. Erster Ordnung	Höherer Ordnung	Pseudomeroedrische Zwillinge s.v. Erster Ordnung	Höherer Ordnung
Hocart's nomenclature (*ca.* 1958)	by merohedry	by reticular merohedry	by pseudo-symmetry crystal lattice	multiple lattice

† The rhombic section is planar, but not a net plane. It contains the twin axis and the line of intersection of the plane perpendicular to the twin axis with the net plane quasi-perpendicular to the twin axis.

††Reported in garnet, haüynite and magnetite:twin plane (210)

§ Black-white symbolism is used to express a single twin law (Curien & Le Corre 1958);a colour group describes the symmetry of the complete twin where several twin laws are involved (Curien & Donnay 1959).

Friedel's classification so that the main subdivisions would be based on the twin obliquity ω rather than on the twin index n. As originally proposed by Friedel, the classification followed the historical development: Bravais ($n = 1$, $\omega = 0$), Mallard ($n = 1$, $\omega > 0$) and Friedel himself ($n > 1$, $\omega = 0$ and $\omega > 0$). It is not clear why Niggli changed the sequence to the one we advocate here: nowhere does he discuss the advantages of the new sequence over the old one from the point of view of the *x*-ray crystallographer, nor does he consider the phenomenon of twinning in reciprocal space.

We must take exception to the term of "merohedry of a higher order" ($\omega = 0$, $n > 1$), as used by Niggli to mean "reticular merohedry" or "lattice merohedry", that is, the situation where the crystal lattice is less symmetrical than one of its "multiple lattices" or "superlattices". The term at issue was proposed by Friedel to designate the case where a crystal lattice or one of its superlattices simulates, as quasi-symmetry with $\omega \sim 0$, the higher symmetry of the lattice of another crystal system. A nice example of this phenomenon is found in staurolite (Hurst *et al.* 1956), monoclinic quasi-orthorhombic, with $\beta = 90°$ within limits of error, which displays twins with $n = 1$ and ω vanishingly small, even though it cannot be rigorously zero. Such twins, in Friedel's terminology, are due to "higher order merohedry"; in Niggli's nomenclature, they would be called "pseudo-merohedral of the first order". It is just as well Niggli's terminology has not made much headway outside German-speaking countries.

The classification taught at the Sorbonne in the nineteen-fifties (Hocart *ca.* 1958) retained Friedel's two subclasses, "by merohedry" ($\omega = 0$, $n = 1$) and "by reticular merohedry" ($\omega = 0$, $n > 1$), but grouped into a single class, "by pseudo-symmetry" ($\omega > 0$) the two cases $n = 1$ and $n > 1$.

The problem of symbolizing twin symmetry, either to define a twin law or to describe the symmetry of the complete twin, has been solved by the application of the black-white or the colour notation, respectively (Curien & Le Corre 1958; Curien & Donnay 1959).† This solution is satisfactory in cases of twinning by twin-lattice symmetry ($\omega = 0$), but its adequacy remains limited in the case of twinning by twin-lattice quasi-symmetry ($\omega > 0$). The example, given in the Table, of the Albite and Pericline laws ($\omega > 0$, $n = 1$) is a case in point. We are here proposing symbols that contain elements of both direct and reciprocal spaces. The symbol $2^{*\prime}/m'$ brings out the fact that the twin operation can be considered a 180° rotation around the reciprocal-lattice row-line [010]*, as well as a reflection in the direct-lattice net-plane (010). Proof of the equivalence of these two twin operations rests on their product being equal to a crystal-symmetry operation — the inversion through the center $\bar{1}$. In accordance with the law of Mallard, for nearly one hundred years now, the twin element has usually been chosen as the direct-lattice element: $m'(010)$ for Albite twinning and $2'[010]$ for Pericline twinning. Some devotees of twinning "by half-turn rotation", however, have kept alive the "axes of hemitropy" of old, which are still commonly used in petrography textbooks. In *x*-ray-diffraction work, particularly by the precession techniques, the twin definition by means of the reciprocal-lattice element has suddenly acquired paramount importance: Albite twinning is detected because the two orientations of the reciprocal lattice are related by a 180° rotation around [010]*, whereas in the Pericline twinning they are reflected in (010)*. Each of the symbols $2^{*\prime}/m'$ and $2''/m^{*\prime\prime}$ describes both the twin law and the twin symmetry, and each one implies the presence of $\bar{1}$. The question arises: is it possible to symbolize the symmetry of the edifice when these two "correspondent twins" (twins due to the quasi-symmetry of one and the same cell) co-exist in one specimen? Is it possible to find here the analogue of the "symmetry of the complete twin", which is usually defined when $\omega = 0$? We have considered describing the complete twin by $\left(\frac{2^{*\prime}}{m'}, \frac{2''}{m^{*\prime\prime}}\right)$, that is, the juxtaposition of the two symbols that represent the Albite and Pericline laws, respectively, but a more compact notation would seem to be preferable. We propose the symbol $\frac{2''}{m'}\ \bar{1}$. It contains only direct-lattice twin elements. The dashed fraction bar is chosen to

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† Errata in Curien & Donnay (1959):
p. 1068, line 11 up: "... Brazil law are double-primed..." should read "... Brazil law are triple-primed..."
p. 1068, line 10 up: "... triple primes..." should read "... double primes..."
In that paper, as in Curien and LeCorre (1958, Fig. 1), the Dauphiné twin comprises crystals (I-II) or (III-IV); the Brazil twin crystals (I-IV) or (II-III), and the D-B twin crystals (I-III) or (II-IV).

mean "nearly perpendicular to", by analogy with the solid fraction bar (now universally accepted), which stands for "rigorously perpendicular to". The co-existence of the Albite twin mirror m' and the Pericline twin axis $2''$ does not imply the center $\bar{1}$, which must therefore be explicitly stated in the new symbol; it is written after the dashed bar. Note that the inversion in $\bar{1}$ can be mentally combined either with the reflection in m' to give $2^{*\prime}$ or with the rotation in $2''$ to yield $m^{*\prime\prime}$.

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