International Tables for Crystallography (2006). Vol. D, Section 3.3.8.5, pp. 420–421.

(*b*) only *two* lattices are superimposed to form the twin lattice.

In the present section these two conditions are relaxed as follows:

(1) In addition to exact lattice coincidences (as they occur for all merohedral twins) *approximate* lattice coincidences (pseudo-coincidences) are taken into account.

In this context, it is important to explain the meaning of the terms *approximate lattice coincidences* or *pseudo lattice coincidences* as used in this section. Superposition of two or more equal lattices (with a common origin) that are slightly misoriented with respect to each other leads to a three-dimensional moiré pattern of coincidences and anti-coincidences. The *beat period* of this pattern increases with decreasing misorientation. It appears sensible to use the term approximate or pseudo-coincidences only if the 'splitting' of lattice points is small within a sufficiently large region around the common origin of the two lattices. Special cases occur for reflection twins and rotation twins of pseudosymmetrical lattices. For the former, exact two-dimensional coincidences exist parallel to the (rational) twin reflection plane and the moiré pattern is only one-dimensional in the direction normal to this plane. Hence, the region of 'small splitting' is a two-dimensional (infinitely extended) thin layer of the twin lattice on both sides of the twin reflection plane [example: pseudo-monoclinic albite (010) reflection twins]. For rotation twins, the region of 'small splitting' is an (infinitely long) cylinder around the twin axis. On the axis the lattice points coincide exactly.

In general, a typical measure of this region, in terms of the reciprocal lattice, could be the size of a conventional X-ray diffraction photograph. Whereas the slightest deviations from exact coincidence lead to pseudo-coincidences, the 'upper limit of the splitting', up to which two lattices are considered as pseudo-coincident, is not definable on physical grounds and thus is a matter of convention and personal preference. As an angular measure of the splitting the *twin obliquity* has been introduced by Friedel (1926). This concept and its use in twinning will be discussed below in Section 3.3.8.5.

(2) The previous treatment of superposition of only two lattices is extended to multiple twins with several interpenetrating lattices which are related by a pseudo n-fold twin axis. Such a twin axis cannot be 'exact', no matter how close its rotation angle comes to the exact angular value. For this reason, twin axes of order $n > 2$ necessarily lead to *pseudo* lattice coincidences.

Here it is assumed that such pseudo-coincidences exist for any pair of neighbouring twin domains. As a consequence, pseudo-coincidences occur for all n domains. For this case, the following rules exist:

(i) Only n-fold twin axes with the crystallographic values $n = 3$, 4 and 6 lead to pseudo lattice coincidences of all domains. Example: cyclic triplets of aragonite.

(ii) The number of (interpenetrating) lattices equals the number of different domain states [*cf.* Section 3.3.4.4(iii)], *viz.*

$$\begin{aligned} 6, 3 \text{ or } 2 \text{ lattices for } n &= 6,\\ 3 \text{ lattices for } n &= 3,\\ 4 \text{ or } 2 \text{ lattices for } n &= 4, \end{aligned}$$

whereby the case '2 lattices' for $n = 6$ leads to exact lattice coincidence (merohedral twinning, *e.g.* Dauphiné twins of quartz).

(iii) There always exists *exact* (one-dimensional) coincidence of all lattice rows along the twin axis.

(iv) If there is a (rational) lattice plane normal to the twin axis, the splitting of the lattice points occurs only parallel to this plane. If, however, this lattice plane is pseudo-normal (*i.e.* slightly inclined) to the twin axis, the splitting of lattice points also has a small component along the twin axis.

3.3.8.5. *Twin obliquity and lattice pseudosymmetry*

The concept of *twin obliquity* has been introduced by Friedel (1926, p. 436) to characterize (metrical) pseudosymmetries of lattices and their relation to twinning. The obliquity ω is defined as the angle between the normal to a given lattice plane (hkl) and a lattice row [uvw] that is not parallel to (hkl) and, *vice versa*, as the angle between a given lattice row [uvw] and the normal to a lattice plane (hkl) that is not parallel to [uvw]. The twin obliquity is thus a quantitative (angular) measure of the pseudosymmetry of a lattice and, hence, of the deviation which the twin lattice suffers in crossing the composition plane (*cf.* Section 3.3.8.1).

The smallest mesh of the net plane (hkl) together with the shortest translation period along [uvw] define a unit cell of a sublattice of lattice index [j]; j may be $= 1$ or > 1 [*cf.* Section 3.3.8.2(iv)]. The quantities ω and j can be calculated for any lattice and any (hkl)/[uvw] combination by elementary formulae, as given by Friedel (1926, pp. 249–252) and by Donnay & Donnay (1972). Recently, a computer program has been written by Le Page (1999, 2002) which calculates for a given lattice all (hkl)/[uvw]/ω/j combinations up to given limits of ω and j. In the theory of Friedel and the French School, a (metrical) pseudosymmetry of a lattice or sublattice is assumed to exist if the twin obliquity ω as well as the twin lattice index j are 'small'. This in turn means that the pair lattice plane (hkl)/lattice row [uvw] is the better suited as twin elements (twin reflection plane/twofold twin axis) the smaller ω and j are.

The term 'small' obviously cannot be defined in physical terms. Its meaning rather depends on conventions and actual analyses of triperiodic twins. In his textbook, Friedel (1926, p. 437) quotes frequently observed twin obliquities of 3–4° (albite 4°3′, aragonite 3°44′) with 'rare exceptions' of 5–6°. In a paper devoted to the quartz twins with 'inclined axes', Friedel (1923, pp. 84 and 86) accepts the La Gardette (Japanese) and the Esterel twins, both with large obliquities of $\omega = 5°27'$ and $\omega = 5°48'$, as pseudo-merohedral twins only because their lattice indices [j] = 2 and 3 are ('*en revanche*') remarkably small. He considers $\omega = 6°$ as a limit of acceptance ['*limite prohibitive*'; Friedel (1923, p. 88)].

Lattice indices [j] = 3 are very common (in cubic and rhombohedral crystals), [j] = 5 twins are rare and [j] = 6 seems to be the maximal value encountered in twinning (Friedel, 1926, pp. 449, 457–464; Donnay & Donnay, 1974, Table 1). In his quartz paper, Friedel (1923, p. 92) rejects all pseudo-merohedral quartz twins with [j] ≥ 4 despite small ω values, and he points out, as proof that high j values are particularly unfavourable for twinning, that strictly merohedral quartz twins with [j] = 7 do not occur, *i.e.* that $\omega = 0$ cannot 'compensate' for high j values.

In agreement with all these results and later experiences (*e.g.* Le Page, 1999, 2002), we consider in Table 3.3.8.2 only lattice pseudosymmetries with $\omega \leq 6°$ and [j] ≤ 6, preferably [j] ≤ 3. (It should be noted that, on purely mathematical grounds, arbitrarily small ω values can always be obtained for sufficiently large values of h, k, l and u, v, w, which would be meaningless for twinning.) The program by Le Page (1999, 2002) enables for the first time systematic calculations of many ('all possible') (hkl)/[uvw] combinations for a given lattice and, hence, statistical and geometrical evaluations of existing and particularly of (geometrically) 'permissible' but not observed twin laws. In Table 3.3.8.2, some examples are presented that bring out both the merits and the problems of lattice geometry for the theory of twinning. The 'permissibility criteria' $\omega \leq 6°$ and [j] ≤ 6, mentioned above, are observed for most cases.

The following comments on these data should be made.

Gypsum: The calculations result in nearly 70 'permissible' (hkl)/[uvw] combinations. For the very common (100) dovetail twin, four (100)/[uvw] combinations are obtained. Only the two combinations with smallest ω and [j] are listed in the table; similarly for the less common (001) Montmartre twin. In addition, two cases of low-index (hkl) planes with small obliquities and small lattice indices are listed, for which twinning has never been observed.

Rutile: Here nearly twenty 'permissible' (*hkl*)/[*uvw*] combinations with $\omega \le 6°$, $[j] \le 6$ occur. For the frequent (101) reflection twins, five permissible cases are calculated, of which two are given in the table. For the rare (301) reflection twins, only the one case listed, with high obliquity $\omega = 5.4°$, is permissible. For the further two cases of low obliquity and lattice index [5], twins are not known. Among them is one case of (strict) 'reticular merohedry', (210) or (130), with $\omega = 0$ and $[j] = 5$ (*cf.* Fig. 3.3.8.1).

Quartz: The various quartz twins with inclined axes were studied extensively by Friedel (1923). The two most frequent cases, the Japanese $(11\bar{2}2)$ twin (called La Gardette twin by Friedel) and the $(10\bar{1}1)$ Esterel twin, are considered here. In both cases, several lattice pseudosymmetries occur. Following Friedel, those with the smallest lattice index, but relatively high obliquity close to 6° are listed in the table. Again, a twin of (strict) 'reticular merohedry' with $\omega = 0$ and $[j] = 7$ does not occur [*cf.* Section 3.3.9.2.3, Example (2)].

Staurolite: Both twin laws occurring in nature, (031) and (231), exhibit small obliquities but rather high lattice indices [6] and [12]. The frequent (231) 60° twin with $[j] = 12$ falls far outside the 'permissible' range. The further two planes listed in the table, (201) and (101), exhibit favourably small obliquities and lattice indices, but do not form twins. The existing (031) and (231) twins of staurolite are discussed again in Section 3.3.9.2 under the aspect of 'reticular pseudo-merohedry'.

Calcite: For calcite, 19 lattice pseudosymmetries obeying Friedel's 'permissible criteria' are calculated. Again, only a few are mentioned here (indices referred to the structural cell). For the primary deformation twin $(01\bar{1}8)$, **e**-twin after Bueble & Schmahl (1999), *cf.* Section 3.3.10.2.2, Example (5), one permissible lattice pseudosymmetry with small obliquity 0.59 but high lattice index [5] is found. For the less frequent secondary deformation twin $(10\bar{1}4)$, **r**-twin, the situation is similar. The planes $(01\bar{1}2)$ and $(10\bar{1}1)$ permit small obliquities and lattice indices $\le [5]$, but do not appear as twin planes.

The discussion of the examples in Table 3.3.8.2 shows that, with one exception [staurolite (231) twin], the obliquities and lattice indices of common twins fall within the $\omega/[j]$ limits accepted for lattice pseudosymmetry. Three aspects, however, have to be critically evaluated:

(i) For most of the lattice planes (*hkl*), several pseudo-normal rows [*uvw*] with different values of ω and [*j*] within the 6°/[6] limit occur, and *vice versa*. Friedel (1923) discussed this in his theory of quartz twinning. He considers the (*hkl*)/[*uvw*] combination with the smallest lattice index as responsible for the observed twinning.

(ii) Among the examples given in the table, low-index (*hkl*)/[*uvw*] combinations with more favourable $\omega/[j]$ values than for the existing twins can be found that never form twins. A prediction of twins on the basis of 'lattice control' alone, characterized by low ω and [*j*] values, would fail in these cases.

(iii) All examples in the table were derived solely from lattice geometry, none from structural relations or other physical factors.

Note. As a mathematical alternative to the term 'obliquity', another more general measure of the deviation suffered by the twin lattice in crossing the twin boundary was presented by Santoro (1974, equation 36). This measure is the difference between the metric tensors of lattice 1 and of lattice 2, the latter after retransformation by the existing or assumed twin operation (or more general orientation operation).

Table 3.3.8.2. *Examples of calculated obliquities ω and lattice indices [j] for selected (hkl)/[uvw] combinations and their relation to twinning*

Calculations were performed with the program *OBLIQUE* written by Le Page (1999, 2002).

Crystal	(*hkl*)	Pseudo-normal [*uvw*]	Obliquity [°]	Lattice index [*j*]	Remark
Gypsum $A2/a$ $a = 6.51$, $b = 15.15$, $c = 6.28$ Å $\beta = 127.5°$	(100)	[302] [805]	2.47 0.42	3 4	Dovetail twin (very frequent)
	(001)	[203] [305]	5.92 0.95	3 5	Montmartre twin (less frequent)
	(101)	[101]	2.60	2	No twin
	$(11\bar{1})$	$[31\bar{4}]$	1.35	4	No twin
Rutile $P4_2/mnm$ $a = 4.5933$, $c = 2.9592$ Å	(101)	[102] [307]	5.02 0.84	3 5	Frequent twin
	(301)	[101]	5.43	2	Rare twin
	(201)	[304]	2.85	5	No twin
	(210) or (130)	[210] or [130]	0	5	No twin
Quartz $P3_121$ $a = 4.9031$, $c = 5.3967$ Å	$(11\bar{2}2)$	[111]	5.49	2	Japanese twin (La Gardette) (rare)
	$(10\bar{1}1)$	[211]	5.76	3	Esterel twin (rare)
	$(10\bar{1}2)$	[212]	5.76	3	Sardinia twin (very rare)
	$(21\bar{3}0)$ or $(14\bar{5}0)$	[540] or [230]	0	7	No twin
Staurolite $C2/m$ $a = 7.781$, $b = 16.620$, $c = 5.656$ Å $\beta = 90.00°$	(031)	[013]	1.19	6	90° twin (rare)
	(231)	[313]	0.90	12	60° twin (frequent)
	(201)	[101]	0.87	3	No twin
	(101)	[102]	0.87	3	No twin
Calcite $R\bar{3}c$ $a = 4.989$, $c = 17.062$ Å [hexagonal axes, structural X-ray cell; *cf.* Section 3.3.10.2.2, Example (5)]	$(01\bar{1}2)$	[5,10,1] [7,14,2] [481]	5.31 2.57 0.59	2 3 5	No twin
	$(10\bar{1}4)$	[421]	0.74	4	Rare deformation twin (**r**-twin)
	$(01\bar{1}8)$	[121]	0.59	5	Frequent deformation twin (**e**-twin)
	$(10\bar{1}1)$	[14.7.1]	1.54	5	No twin