*International Tables for Crystallography* (2006). Vol. D, Section 3.3.8.4, pp. 419–420.



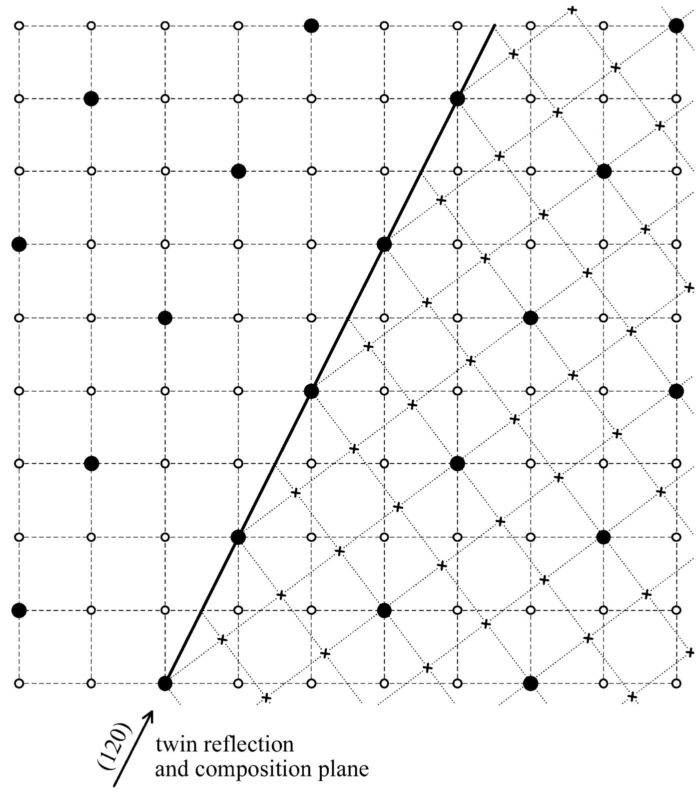


Fig. 3.3.8.1. Lattice relations of $\Sigma 5$ twins of tetragonal crystals with primitive lattice: twin mirror plane and composition plane (120) with twin displacement vector $\mathbf{t} = \mathbf{0}$. Small dots: lattice points of domain 1; small x: lattice points of domain 2; large black dots: $\Sigma 5$ coincidence lattice.

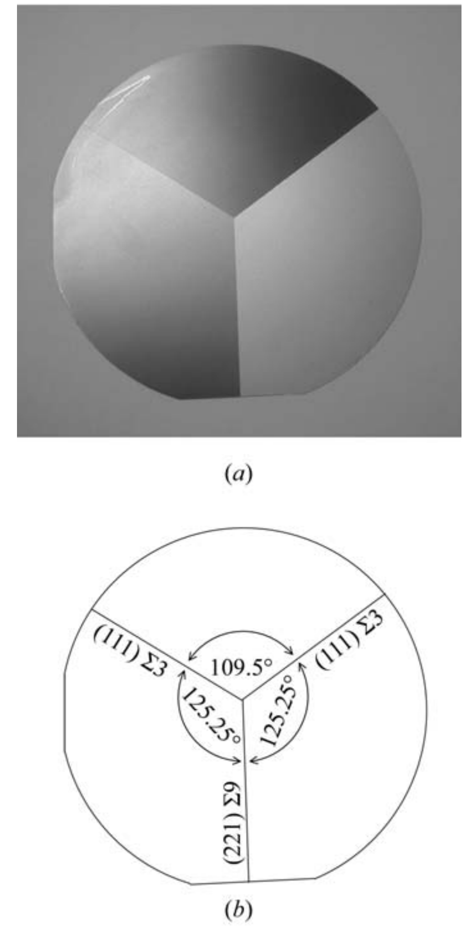


Fig. 3.3.8.2. (*a*) A (110) silicon slice (10 cm diameter, 0.3 mm thick), cut from a Czochralski-grown tricrystal for solar-cell applications. As seed crystal, a cylinder of three coalesced Si single-crystal sectors in (111) and (221) reflection-twin positions was used. Pulling direction [110] (Courtesy of M. Krühler, Siemens AG, München). (*b*) Sketch of the tricystal wafer showing the twin relations [twin laws $m(111)$ and $m(221)$] and the $\Sigma$ characters of the three domain pairs. The atomic structures of these (111) and (221) twin boundaries are discussed by Kohn (1956, 1958), Hornstra (1959, 1960) and Queisser (1963).

to $[j] = 13$. Later structural studies, however, suggest the possibility of disorder instead of twinning.

(4) *Galena, PbS* (NaCl structure). Galena crystals from various localities often exhibit lamellae parallel to the planes {441} which are interpreted as (441) reflection twins with $[j] = 33$ ($\Sigma 33$ twin) (*cf.* Niggli, 1926, Fig. 9k on p. 53). These natural twins are deformation and not growth twins. In laboratory deformation experiments, however, these twins could not be generated. A detailed analysis of twinning in PbS with respect to plastic deformation is given by Seifert (1928).

(5) For cubic metals and alloys *annealing twins* (*recrystallization twins*) with $[j] > 3$ are common. Among them *high-order twins* (*high-generation twins*) are particularly frequent. They are based on the $\Sigma 3$ (spinel) twins (first generation) which may coalesce and form 'new twins' with $\Sigma 9 = 3^2$ [second generation, with twin reflection plane (221)], $\Sigma 27 = 3^3$ [third generation, twin reflection plane (115)], $\Sigma 81 = 3^4$ [fourth generation, twin reflection plane (447)] *etc.* Every step to a higher generation increases $\Sigma$ by a factor of three (Gottstein, 1984). An interesting and actual example is the artificial silicon *tricrystal* shown in Fig. 3.3.8.2, which contains three components related by two (111) reflection planes (first generation, two $\Sigma 3$ boundaries) and one (221) reflection plane (second generation, one $\Sigma 9$ boundary).

(6) The same type of tricrystal has been found in cubic magnetite ($Fe_3O_4$) nanocrystals grown from the biogenic action of magnetotactic bacteria in an aquatic environment (Devouard *et al.*, 1998). Here, HRTEM micrographs (Fig. 6 of the paper) show the same triple-twin arrangement as in the Si tricrystal above. The authors illustrate this triple twin by (111) spinel-type intergrowth of three octahedra exhibiting two $\Sigma 3$ and one $\Sigma 9$ domain pairs. The two $\Sigma 3$ interfaces are (111) twin reflection planes, whereas the $\Sigma 9$ boundary is very irregular and not a compatible planar (221) interface (*i.e.* not a twin reflection plane).

(7) A third instructive example is provided by the fivefold cyclic 'cozonal' twins (zone axis $[1\bar{1}0]$) of Ge nanocrystals (Neumann *et al.*, 1996; Hofmeister, 1998), which are treated in Section 3.3.10.6.5 and Fig. 3.3.10.11. All five boundaries between neighbouring domains (sector angles 70.5°) are of the $\Sigma 3(111)$ type. Second nearest ($2 \times 70.5°$), third nearest ($3 \times 70.5°$) and fourth nearest ($4 \times 70.5°$) neighbours exhibit $\Sigma 9$, $\Sigma 27$ and $\Sigma 81$ coincidence relations (second, third and fourth $\Sigma$ generation), respectively, as introduced above in (5). These relations can be described by the 'cozonal' twin reflection planes (111), (221), (115) and (447). Since $5 \times 70.5° = 352.5°$, an angular gap of 7.5° would result. In actual crystals this gap is compensated by stacking faults as shown in Fig. 3.3.10.11. A detailed treatment of all these cases, including structural models of the interfaces, is given by Neumann *et al.* (1996).

(8) Examples of (hypothetical) twins with $[j] > 1$ due to metrical specialization of the lattice are presented by Koch (1999).

### 3.3.8.4. *Approximate (pseudo-)coincidences of two or more lattices*

In part (iv) of Section 3.3.8.2, three-dimensional lattice coincidences and twin lattices (sublattices) were considered under two restrictions:

(*a*) the lattice coincidences (according to the twin lattice index $[j]$) are *exact* (not approximate);

 

(*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 $\omega$ 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 $\omega$ 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 $(hkl)/[uvw]/\omega/j$ combinations up to given limits of $\omega$ 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 $\omega$ 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 $\omega$ 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 $[j] \geq 4$ despite small $\omega$ 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 $[j] \leq 6$, preferably $[j] \leq 3$. (It should be noted that, on purely mathematical grounds, arbitrarily small $\omega$ 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 $[j] \leq 6$, 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 $\omega$ 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