International Tables for Crystallography (2006). Vol. C, Section 1.3.2, pp. 10–12.

1.3. Twinning

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1.3.1. General remarks

A twin consists of two or more single crystals of the same species but in different orientation, its *twin components*. They are intergrown in such a way that at least some of their lattice directions are parallel. The *twin law* describes the geometrical relation between the twin components. It specifies a symmetry operation, the *twin operation*, that brings one of the twin components into parallel orientation with the other. The corresponding symmetry element is called the *twin element*.

There are several kinds of twin laws:

(1) *Reflection twins*. Two twin components are related by reflection through a net plane (*hkl*), the *twin plane*. All lattice vectors parallel to (*hkl*), *i.e.* a complete lattice plane, coincide for both twin components, and their crystal faces (*hkl*) [and ($\bar{h}\bar{k}\bar{l}$)] are parallel. As a consequence, their corresponding zone axes parallel to (*hkl*) also coincide.

A twin plane cannot run parallel to a mirror or glide plane of the crystal structure, *i.e.* it cannot run parallel to a mirror plane of the point group of the crystal, because in that case both twin components would have the same orientation.

It must be noted that the vector normal to a twin plane need not have rational indices nor be parallel to a lattice vector.

(2) *Rotation twins*. The twin components can be brought into parallel orientation by a rotation about an axis, the *twin axis*. Two cases may be distinguished:

(i) Most frequently, the twin axis runs parallel to a lattice vector with components u, v, w. Then the lattice row [*uvw*] coincides for all twin components, *i.e.* they have the common zone axis [*uvw*]. Usually, the twin axis is a twofold axis, and all corresponding crystal faces of the two twin components belonging to that zone are parallel. Less frequently, a three-, four-, or sixfold rotation occurs as the twin operation.

A twin axis cannot run parallel to a (screw-) rotation axis of the crystal structure which induces the same rotation angle, *i.e.* it cannot be parallel to such a rotation axis of the point group of the crystal. For example, a twofold twin axis cannot be parallel to a twofold, fourfold, or sixfold axis, but it may run parallel to a threefold axis; a twin axis with rotation angle 60, 90, or 120°, however, may be parallel to a twofold axis.

(ii) In some cases, the direction of the twin axis is not rational, but the twofold twin axis runs perpendicular to a lattice row (zone axis) [*uvw*] and parallel to a net plane (crystal face) (*hkl*) that belongs to that zone. Then the lattices of the twin components coincide only in one lattice row parallel to [*uvw*], and [*uvw*] is the common zone axis of both twin components. The crystal faces (*hkl*) and ($\bar{h}\bar{k}\bar{l}$) are parallel for both components, but the other faces of the zone [*uvw*] are not.

Neither in case (i) nor in case (ii) does the plane perpendicular to the twin axis need to be a lattice plane. Therefore, in general, it cannot be described by Miller indices.

(3) *Inversion twins*. The twin components are related by inversion through a centre of symmetry, the *twin centre*. Only noncentrosymmetrical crystals can form such twins. As all corresponding lattice vectors of the two twin components are antiparallel, their entire vector lattices coincide. As a consequence, all corresponding zone axes and crystal faces of the twin components are parallel.

In many cases, there does not exist a unique twin law, but a twin may be described equally well by more than one twin law. (*a*) If the crystal structure of the twin components contains an evenfold rotation or screw-rotation axis, an inversion twin cannot be distinguished from a reflection twin with twin plane perpendicular to that axis. (*b*) If the crystal structure contains a mirror or a glide plane, an inversion twin cannot be distinguished from a rotation twin with a twofold twin axis perpendicular to that plane. (*c*) If for a centrosymmetrical crystal structure the normal of a twin plane runs parallel to a lattice vector or a twin axis runs perpendicular to a net plane, the twin may be described equally well as a reflection twin or as a rotation twin.

The twin components are grown together in a surface called *composition surface*, *twin interface* or *twin boundary*. In most cases, the composition surfaces are low-energy surfaces with good structural fit. For a reflection twin, it is usually a plane parallel to the twin plane. The composition surface of a rotation twin may either be a plane parallel to the twin axis or be a non-planar surface with irregular shape.

If more than two components are twinned according to the same law, the twin is called a *repeated twin* or a *multiple twin*. If all the twin boundaries are parallel planes, it is a *polysynthetic twin*, otherwise it is called a *cyclic twin*. If the twin components are related to each other by more than one twin law, the shape and the mutual arrangement of the twin domains may be very irregular.

With respect to the formation process, one may distinguish between *growth twins*, *transformation twins*, and *mechanical* (*deformation, glide*) *twins*. Transformation twins result from phase transitions, *e.g.* of ferroelectric or ferromagnetic crystals. The corresponding twin domains are usually small and the number of such domains is high. Mechanical twinning is due to mechanical stress and may often be described in terms of shear of the crystal structure. This includes ferroelasticity.

Twins are observable by, for example, macroscopic or microscopic observation of re-entrant angles between crystal faces, by etching, by means of different extinction positions for the twin components between cross polarizers of a polarization microscope, by different rotation angles of the plane of polarization of a beam of plane-polarized light passing through the components of a twin showing optical activity, by a splitting of part of the X-ray diffraction spots (except for twins by merohedry), by means of domain contrast or boundary contrast in an X-ray topogram, or by investigation with a transmission electron microscope.

The phenomenon of twinning has frequently been described and discussed in the literature and it is impossible, therefore, to give a complete list of references. Further details may be learned, *e.g.* from a review article by Cahn (1954) or from appropriate textbooks. A comprehensive survey of X-ray topography of twinned crystals is given by Klapper (1987). The following papers are related to twinning by merohedry or pseudo-merohedry: Catti & Ferraris (1976), Grimmer (1984, 1989*a*,*b*), Grimmer & Warrington (1985), Donnay & Donnay (1974), Le Page, Donnay & Donnay (1984), Hahn (1981, 1984), Klapper, Hahn & Chung (1987), Flack (1987).

1.3.2. Twin lattices

For reflection and rotation twins described in the last section, a special situation arises whenever there exists a lattice vector perpendicular to the twin plane or a lattice plane perpendicular to

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Table 1.3.2.1. *Lattice planes and rows that are perpendicular to each other independently of the metrical parameters*

Basis system	Lattice plane (hkl)	Lattice row $[uvw]$	Perpendicularity condition
Triclinic	–	–	–
Monoclinic (unique axis **b**)	(010)	[010]	–
Monoclinic (unique axis **c**)	(001)	[001]	–
Orthorhombic	(100) (010) (001)	[100] [010] [001]	– – –
Hexagonal/ trigonal	$(hk0)$ (001)	$[uv0]$ [001]	$u = 2h + k$, $v = h + 2k$ –
Rhombohedral	$(h, k, -h - k)$ (111)	$[u, v, -u - v]$ [111]	$u = h, v = k$ –
Tetragonal	$(hk0)$ (001)	$[uv0]$ [001]	$u = h, v = k$ –
Cubic	(hkl)	$[uvw]$	$u = h, v = k, w = l$

a rational twofold twin axis. Such a situation occurs systematically for all reflection and rotation twins with cubic symmetry and for certain twins with non-cubic symmetry (*cf.* Table 1.3.2.1). In addition, such a perpendicularity may occur occasionally if equation (1.1.2.12) is satisfied.

In the case of a noncentrosymmetric crystal structure, different twins result from a twin axis $[uvw]$ with a perpendicular lattice plane (hkl), or from a twin plane (hkl) with a perpendicular lattice row $[uvw]$: the reflection twin consists of two enantiomorphous twin components whereas the rotation twin is built up from two crystals with the same handedness (*cf.*, for example, Brazil twins and Dauphiné twins of quartz). With respect to the first twin component, the lattice of the second component has the same orientation in both cases. For a centrosymmetrical crystal structure, both twin laws give rise to the same twin.

Whenever a twin plane or twin axis is perpendicular to a lattice vector or a net plane, respectively, the vector lattices of the twin components have a three-dimensional subset in common. This sublattice [derivative lattice, *cf. IT* A (1983, Chapter 13.2)] is called the *twin lattice*. It corresponds uniquely to the intersection group of the two translation groups referring to the twin components. The respective subgroup index i is called the *twin index*. It is equal to the ratio of the volumes of the primitive unit cells for the twin lattice and the crystal structure. If one subdivides the crystal lattice into nets parallel to the twin plane or perpendicular to the twin axis, each ith of these nets belongs to the common twin lattice of the two twin components (*cf.* Fig. 1.3.2.1). Important examples are cubic twins with [111] as twofold twin axis or (111) as twin plane and rhombohedral twins with [001] as twin axis or (001) as twin plane (hexagonal description). In all these cases, the twin index i equals 3.

For every twin lattice, its twin index i can be calculated from the Miller indices of the net plane (hkl) and the coprime coefficients u, v, w of the lattice vector $\mathbf{t}$ perpendicular to (hkl). Referred to a primitive lattice basis, i is simply related to the modulus of the scalar product j of the two vectors $\mathbf{r}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$ and $\mathbf{t} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$:

$$j = \mathbf{r}^* \cdot \mathbf{t} = hu + kv + lw,$$

$$i = \begin{cases} |j| & \text{for } j = 2n + 1 \\ |j|/2 & \text{for } j = 2n \end{cases} \qquad (n \text{ integer}).$$

The same procedure – but with modified coefficients – may be applied to a centred lattice described with respect to a conventionally chosen basis: The coprime Miller indices h, k, l that characterize the net plane have to be replaced by larger non-coprime indices h', k', l', if h, k, l do not refer to a (non-extinct) point of the reciprocal lattice. The integer coefficients u, v, w specifying the lattice vector perpendicular to (hkl) have to be replaced by smaller non-integer coefficients u', v', w', if the centred lattice contains such a vector in the direction $[uvw]$.

1.3.2.1. *Examples*

(1) Cubic P lattice: [111] is perpendicular to (111).
$j = hu + kv + lw = 3$ odd
$i = |j| = 3$.

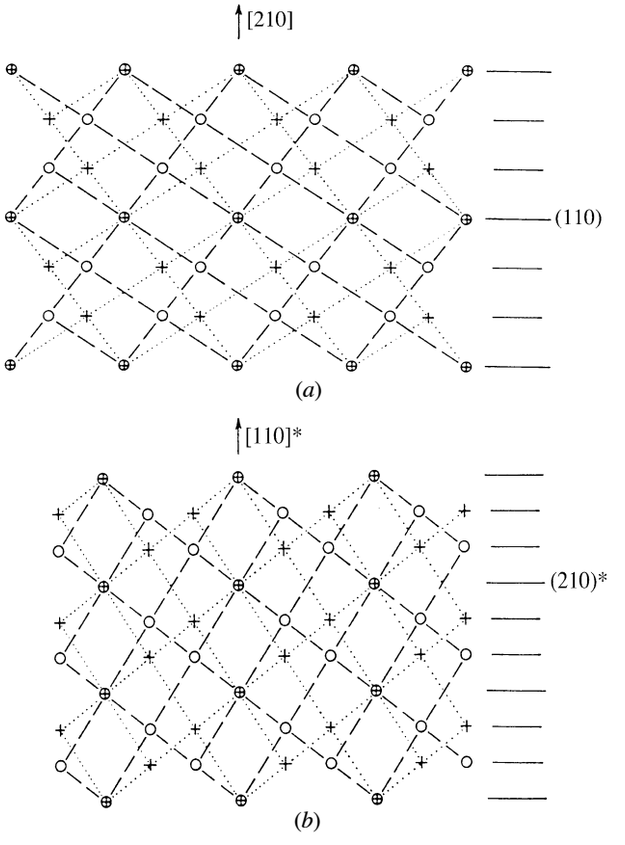

Fig. 1.3.2.1. (*a*) Projection of the lattices of the twin components of a monoclinic twinned crystal (unique axis **c**, $\gamma = 93°$) with twin index 3. The twin may be interpreted either as a rotation twin with twin axis [210] or as a reflection twin with twin plane (110). (*b*) Projection of the corresponding reciprocal lattices.

(2) Orthorhombic lattice with $b = \sqrt{3}a$: [310] is perpendicular to (110).

(i) *P* lattice (*cf.* Fig. 1.3.2.2):
$j = hu + kv + lw = 4$ even
$i = |j|/2 = 2$.

(ii) *C* lattice (*cf.* also Fig. 1.3.2.2):
Because of the *C* centring, [310] has to be replaced by $[\frac{3}{2}\frac{1}{2}0]$.
$j = hu' + kv' + lw' = 2$ even
$i = |j|/2 = 1$.

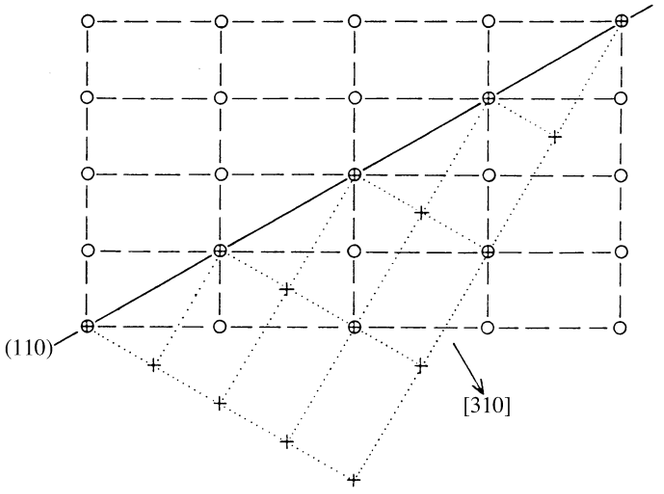

Fig. 1.3.2.2. Projection of the lattices of the twin components of an orthorhombic twinned crystal ($oP, b = \sqrt{3}a$) with twin index 2. The twin may be interpreted either as a rotation twin with twin axis [310] or as a reflection twin with twin plane (110). The figure shows, in addition, that twin index 1 results if the *oP* lattice is replaced by an *oC* lattice in this example (twinning by pseudomerohedry).

(3) Orthorhombic *C* lattice with $b = 2a$: [210] is perpendicular to (120) (*cf.* Fig. 1.3.2.3).
As (120) refers to an 'extinct reflection' of a *C* lattice, the triplet 240 has to be used in the calculation.
$j = h'u + k'v + l'w = 8$ even
$i = |j|/2 = 4$.

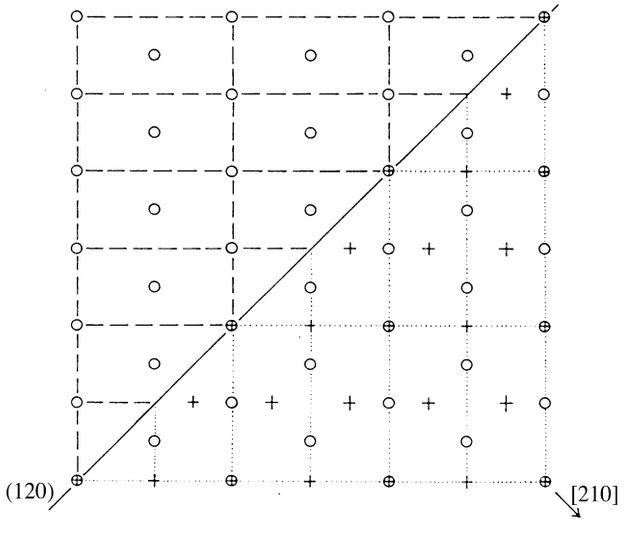

Fig. 1.3.2.3. Projection of the lattices of the twin components of an orthorhombic twinned crystal ($oC, b = 2a$) with twin index 4. The twin may be interpreted either as a rotation twin with twin axis [210] or as a reflection twin with twin plane (120).

(4) Rhombohedral lattice in hexagonal description with $c = \frac{1}{2}\sqrt{3}a$: $[\bar{1}1\bar{2}]$ is perpendicular to $(1\bar{1}1)$.
Because of the *R* centring, $[\bar{1}1\bar{2}]$ has to be replaced by $[\bar{\frac{1}{3}}\frac{1}{3}\bar{\frac{2}{3}}]$.
As $(1\bar{1}1)$ refers to an 'extinct reflection' of an *R* lattice, the triplet $1\bar{1}1$ has to be replaced by $3\bar{3}3$.
$j = h'u' + k'v' + l'w' = -4$ even
$i = |j|/2 = 2$.

1.3.3. Implication of twinning in reciprocal space

As shown above, the direct lattices of the components of any twin coincide in at least one row. The same is true for the corresponding reciprocal lattices. They coincide in all rows perpendicular to parallel net planes of the direct lattices.

For a reflection twin with twin plane (*hkl*), the reciprocal lattices of the twin components have only the lattice points with coefficients *nh*, *nk*, *nl* in common.

For a rotation twin with twofold twin axis [*uvw*], the reciprocal lattices of the twin components coincide in all points of the plane perpendicular to [*uvw*], *i.e.* in all points with coefficients *h*, *k*, *l* that fulfil the condition $hu + kv + lw = 0$.

For a rotation twin with irrational twin axis parallel to a net plane (*hkl*), only reciprocal-lattice points with coefficients *nh*, *nk*, *nl* are common to both twin components.

As the entire direct lattices of the two twin components coincide for an inversion twin, the same must be true for their reciprocal lattices.

For a reflection or rotation twin with a twin lattice of index *i*, the corresponding reciprocal lattices, too, have a sublattice with index *i* in common (*cf*. Fig. 1.3.2.1*b*). In analogy to direct space, the twin lattice in reciprocal space consists of each *i*th lattice plane parallel to the twin plane or perpendicular to the twin axis. If the twin index equals 1, the entire reciprocal lattices of the twin components coincide.

If for a reflection twin there exists only a lattice row [*uvw*] that is almost (but not exactly) perpendicular to the twin plane (*hkl*), then the lattices of the two twin components nearly coincide in a three-dimensional subset of lattice points. The corresponding misfit is described by the quantity ω, the *twin obliquity*. It is the angle between the lattice row [*uvw*] and the direction perpendicular to the twin plane (*hkl*). In an analogous way, the twin obliquity ω is defined for a rotation twin. If (*hkl*) is a net plane almost (but not exactly) perpendicular to the twin axis [*uvw*], then ω is the angle between [*uvw*] and the direction perpendicular to (*hkl*).

1.3.4. Twinning by merohedry

A twin is called a *twin by merohedry* if its twin operation belongs to the point group of its vector lattice, *i.e.* to the corresponding holohedry. As each lattice is centrosymmetric, an inversion twin is necessarily a twin by merohedry. Only crystals from merohedral (*i.e.* non-holohedral) point groups may form twins by merohedry; 159 out of the 230 types of space groups belong to merohedral point groups.

For a twin by merohedry, the vector lattices of all twin components coincide in direct *and* in reciprocal space. The twin index is 1. The maximal number of differently oriented twin components equals the subgroup index *m* of the point group of the crystal with respect to its holohedry.

Table 1.3.4.1 displays all possibilities for twinning by merohedry. For each holohedral point group (column 1), the types of Bravais lattices (column 2) and the corresponding merohedral point groups (column 3) are listed. Column 4 gives the subgroup index *m* of a merohedral point group in its