

## 1.3. TWINNING

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 $\mathbf{b}$ )	(010)	[010]	-
Monoclinic (unique axis $\mathbf{c}$ )	(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  $i$ th 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  $\mathbf{t} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$ :

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

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

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).

$$j = hu + kv + lw = 3 \quad \text{odd}$$

$$i = |j| = 3.$$

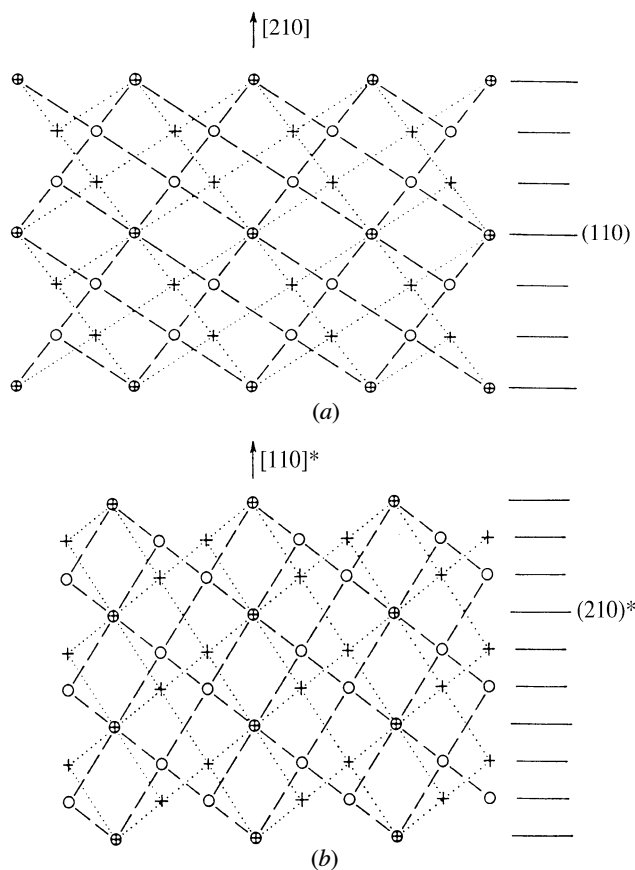


Fig. 1.3.2.1. (a) Projection of the lattices of the twin components of a monoclinic twinned crystal (unique axis  $\mathbf{c}$ ,  $\gamma = 93^\circ$ ) with twin index 3. The twin may be interpreted either as a rotation twin with twin axis [210] or as a reflection twin with twin plane (110). (b) Projection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

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

(i)  $P$  lattice (cf. Fig. 1.3.2.2):

$$j = hu + kv + lw = 4 \quad \text{even}$$

$$i = |j|/2 = 2.$$

(ii)  $C$  lattice (cf. also Fig. 1.3.2.2):

Because of the  $C$  centring,  $[310]$  has to be replaced by  $[\frac{3}{2}10]$ .

$$j = hu' + kv' + lw' = 2 \quad \text{even}$$

$$i = |j|/2 = 1.$$

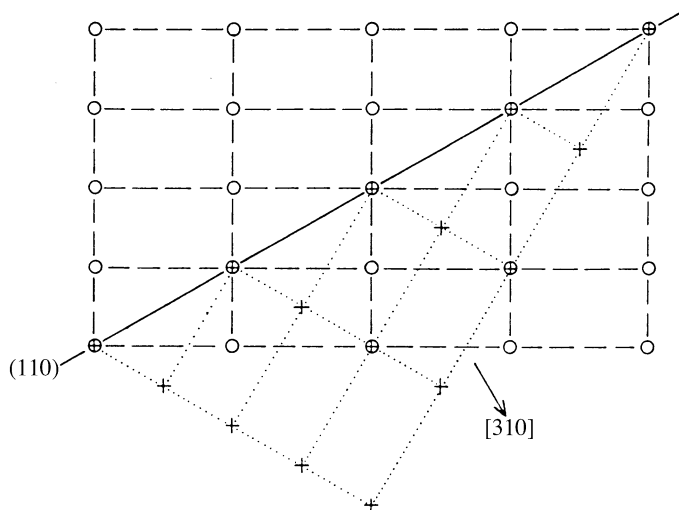


Fig. 1.3.2.2. Projection of the lattices of the twin components of an orthorhombic twinned crystal ( $oP$ ,  $b = \sqrt{3}a$ ) with twin index 2. The twin may be interpreted either as a rotation twin with twin axis  $[310]$  or as a reflection twin with twin plane  $(110)$ . The figure shows, in addition, 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.

$$j = h'u + k'v + l'w = 8 \quad \text{even}$$

$$i = |j|/2 = 4.$$

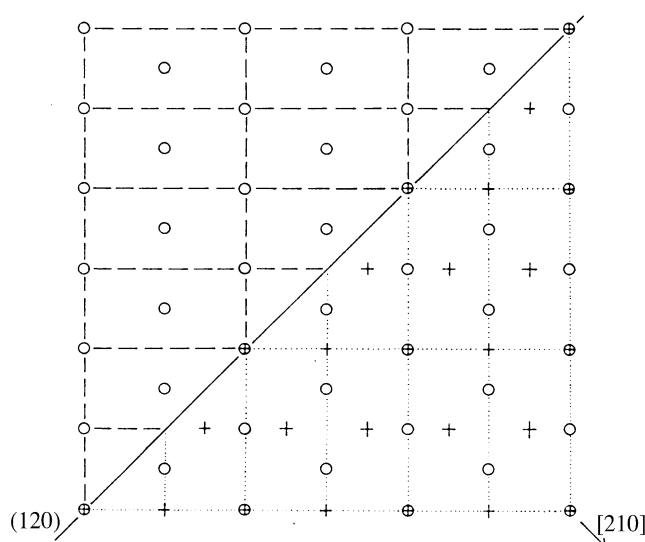


Fig. 1.3.2.3. Projection of the lattices of the twin components of an orthorhombic twinned crystal ( $oC$ ,  $b = 2a$ ) with twin index 4. The twin may be interpreted either as a rotation twin with twin axis  $[210]$  or as a reflection twin with twin plane  $(120)$ .

(4) Rhombohedral lattice in hexagonal description with  $c = \frac{1}{2}\sqrt{3}a$ :  $[\bar{1}12]$  is perpendicular to  $(\bar{1}11)$ .

Because of the  $R$  centring,  $[\bar{1}12]$  has to be replaced by  $[\frac{1}{3}\frac{1}{3}\frac{2}{3}]$ .

As  $(\bar{1}11)$  refers to an 'extinct reflection' of an  $R$  lattice, the triplet  $\bar{1}11$  has to be replaced by  $3\bar{3}3$ .

$$j = h'u' + k'v' + l'w' = -4 \quad \text{even}$$

$$i = |j|/2 = 2.$$

### 1.3.3. Implication of twinning in reciprocal space

As shown above, the direct lattices of the components of a 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. 1.3.2.1b). 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  $\omega$ , 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  $\omega$  is defined for a rotation twin. If  $(hkl)$  is a net plane almost (but not exactly) perpendicular to the twin axis  $[uvw]$ , then  $\omega$  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