

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).

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

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

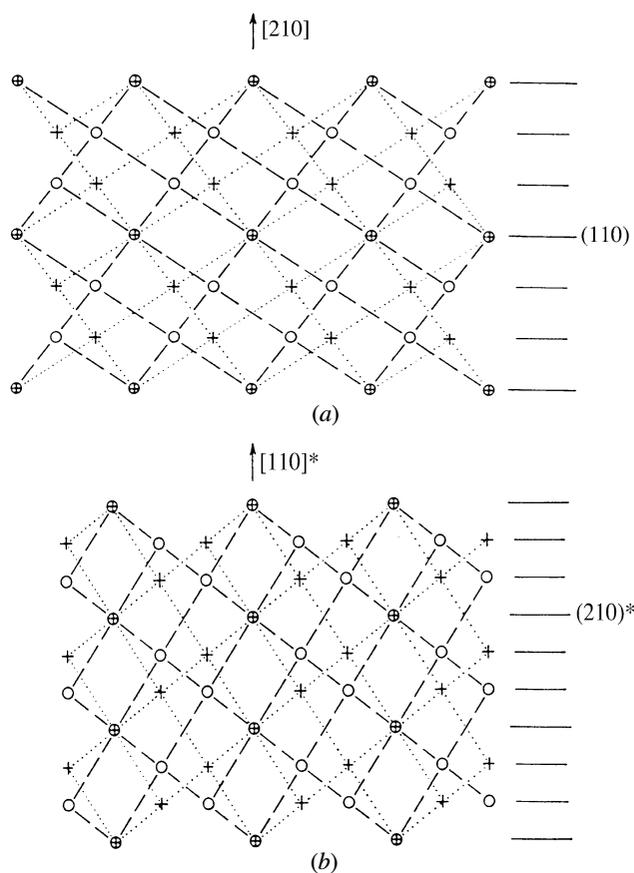


Fig. 1.3.2.1. (a) Projection of the lattices of the twin components of a monoclinic twinned crystal (unique axis \mathbf{c} , $\gamma = 93^\circ$) with twin index 3. The twin may be interpreted either as a rotation twin with twin axis [210] or as a reflection twin with twin plane (110). (b) Projection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