Table 3.3.8.1. *Lattice planes (hkl) and lattice rows [uvw] that are mutually perpendicular (after Koch, 1999)*

Lattice	Lattice plane (*hkl*)	Lattice row [*uvw*]	Perpendicularity condition and quantity $j' = hu + kv + lw$
Triclinic	–	–	–
Monoclinic (unique axis *b*)	(010)	[010]	–
Monoclinic (unique axis *c*)	(001)	[001]	–
Orthorhombic	(100) (010) (001)	[100] [010] [001]	– – –
Hexagonal and rhombohedral (hexagonal axes)	(*hki*0) (0001)	[*uv*0] [001]	$u = 2h + k, v = h + 2k, j' = 2h^2 + 2k^2 + 2hk$ –
Rhombohedral (rhombohedral axes)	$(h, k, -h - k)$ (111)	$[u, v, -u - v]$ [111]	$u = h, v = k, j' = 2h^2 + 2k^2 + 2hk$ –
Tetragonal	(*hk*0) (001)	[*uv*0] [001]	$u = h, v = k, j' = h^2 + k^2$ –
Cubic	(*hkl*)	[*uvw*]	$u = h, v = k, w = l; j' = h^2 + k^2 + l^2$

$$j' = hu + kv + lw \quad (\text{scalar product } \mathbf{r}^{\star}_{hkl} \cdot \mathbf{t}_{uvw})$$

with sublattice index

$$[j] = |j'| \text{ for } j' = 2n + 1$$
$$= |j'|/2 \text{ for } j' = 2n.$$

Here, the indices of the plane (*hkl*) and of the perpendicular row [*uvw*] are referred to a primitive lattice basis (primitive cell). For centred lattices, described by conventional bases, modifications are required; these and further examples are given by Koch (1999). Formulae and tables are presented by Friedel (1926, pp. 245–252) and by Donnay & Donnay (1972). The various equations for the quantity j' are also listed in the last column of Table 3.3.8.1.

Note that in the tetragonal system for any (*hk*0) reflection twin and any [*uv*0] twofold rotation twin, the coincidence lattices are also tetragonal and have the same lattice parameter *c*. Further details are given by Grimmer (2003). An analogous relation applies to the hexagonal crystal family for (*hki*0) and [*uv*0] twins. In the cubic system, the following types of twin lattices occur:

(111) and [111] twins: hexagonal *P* lattice (*e.g.* spinel twins);
(*hk*0) and [*uv*0] twins: tetragonal lattice;
(*hhl*) and [*uuw*] twins: orthorhombic lattice;
(*hkl*) and [*uvw*] twins: monoclinic lattice.

Note that triclinic twin lattices are not possible for a cubic lattice.

After these general considerations of coincidence-site and twin lattices and their lattice index, specific cases of 'triperiodic twins' are treated in Section 3.3.8.3. In addition to the characterization of the twin lattice by its index [*j*], the Σ notation used in metallurgy is included.

3.3.8.3. *Twins with three-dimensional twin lattices ('triperiodic' twins)*

The following cases of exact superposition are distinguished:

(i) *Twins with* $[j] = 1$ ($\Sigma 1$ *twins*). Here, the crystal lattice and the twin lattice are identical, *i.e.* the coincidence (parallelism) of the two oriented crystal lattices is complete. Hence, any twin operation must be a symmetry operation of the point group of the lattice (holohedry), but not of the point group of the crystal. Consequently, this twinning can occur in 'merohedral' point groups only. This *twinning by merohedry* (*parallel-lattice twins*, *twins with parallel axes*) will be treated extensively in Section 3.3.9.

(ii) *Twins with* $[j] = 2$ ($\Sigma 2$ *twins*). This twinning does not occur systematically among the cases listed in Table 3.3.8.1, except for special metrical relations. Example: a primitive orthorhombic lattice with $b/a = \sqrt{3}$ and twin reflection plane (110) or $(\bar{1}10)$. The coincidence lattice is hexagonal with $a_{\rm hex} = 2a$ and $[j] = 2$.

(iii) *Twins with* $[j] = 3$ ($\Sigma 3$ *twins*). Twins with $[j] = 3$ are very common among rhombohedral and cubic crystals ('spinel law') with the following two representative twin operations:

(*a*) twofold rotation around a threefold symmetry axis [111] (cubic or rhombohedral coordinate axes) or [001] (hexagonal axes);

(*b*) reflection across the plane (111) or (0001) normal to a threefold symmetry axis.

Both twin operations belong to the same twin law if the crystal is centrosymmetric. Well known examples are the (0001) contact twins of calcite, the penetration twins of iron borate, $FeBO_3$, with the calcite structure, and the spinel twins of cubic crystals (*cf.* Examples 3.3.6.5, 3.3.6.6 and Figs. 3.3.6.4–3.3.6.6). For crystals with a rhombohedral (*R*) lattice, the coincidence lattice is the primitive hexagonal (*P*) sublattice (whose unit cell is commonly used for the hexagonal description of rhombohedral crystals). Here, the two centring points inside the triple hexagonal *R* cell do not belong to the coincidence sublattice which is, hence, of index $[j] = 3$. The same holds for the spinel twins of cubic crystals, provided only one of the four threefold axes is involved in the twinning.

(iv) *Twins with* $[j] > 3$ ($\Sigma > 3$ *twins*). Whereas twins with $[j] = 3$ are very common and of high importance among minerals and metals, twins with higher lattice indices occur hardly at all. All these 'high-index' twins can occur systematically only in tetragonal, hexagonal, rhombohedral and cubic crystals, due to the geometric perpendicularity relations set out in Table 3.3.8.1. Note that for special lattice metrics (axial ratios and angles) they can occur, of course, in any crystal system. These special metrics, however, are not enforced by the crystal symmetry and hence the coincidences are not strict, but only 'pseudo-coincidences'.

Examples

(1) Tetragonal twins with twin reflection planes {210} or {130}, or twofold twin axes ⟨210⟩ or ⟨130⟩ lead to $[j] = 5$, the largest value of [*j*] that has been found so far for tetragonal twins. The coincidence lattice is again tetragonal with $\mathbf{a}' = 2\mathbf{a} + \mathbf{b}$, $\mathbf{b}' = -\mathbf{a} + 2\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$ and is shown in Fig. 3.3.8.1. An actual example, $SmS_{1.9}$ (Tamazyan *et al.*, 2000*b*), is discussed in Section 3.3.9.2.4.

(2) There exist several old and still unsubstantiated indications for a $[j] = 5$ *cubic garnet twin* with twin reflection plane (210), *cf.* Arzruni (1887); Tschermak & Becke (1915, p. 594).

(3) *Klockmannite, CuSe* (Taylor & Underwood, 1960; Takeda & Donnay, 1965). This hexagonal mineral seems to be the only example for a hexagonal twin with $[j] > 3$. X-ray diffraction experiments indicate a reflection twin on $(13\bar{4}0)$, corresponding