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see Section 3.3.8.2 below. These concepts were further developed by Niggli (1919, 1920/1924/1941).

The lattice aspects of twinning (*triperiodic twins*) are discussed in this section and in Section 3.3.9. An important concept in this field is the *coincidence-site sublattice* of the twin in direct space and its counterpart in reciprocal space. Extensive use of the notion of coincidence-site lattices (CSLs) is made in *bicrystallography* for the study of grain boundaries, as briefly explained in Section 3.2.2.

The coincidence-site lattice and further related lattices (O- and DSC-lattices) were introduced into the study of bicrystals by Bollmann (1970, 1982) and were theoretically thoroughly developed by Grimmer (1989, 2003). Their applications to grain boundaries are contained in the works by Sutton & Balluffi (1995) and Gottstein & Shvindlerman (1999).

3.3.8.1. *Basic concepts of Friedel's lattice theory*

The basis of Friedel's (1904, 1926) lattice theory of twinning is the postulate that the coincidence-site sublattice common to the two twin partners (twin lattice) suffers no deviation (strict condition) or at most a slight deviation (approximate condition) in crossing the boundary between the two twin components (composition plane). This purely geometrical condition is often expressed as 'three-dimensional lattice control' (Santoro, 1974, p. 225), which is supposed to be favourable to the formation of twins.

In order to define the coincidence sublattice (twin lattice) of the two twin partners, it is assumed that their oriented point lattices are infinitely extended and interpenetrate each other. The lattice classification of twins is based on the degree of coincidence of these two lattices. The criterion applied is the dimension of the *coincidence-site subset* of the two interpenetrating lattices, which is defined as the set of all lattice points common to both lattices, provided that two initial points, one from each lattice, are brought to coincidence (common origin). This common origin has the immediate consequence that the concept of the twin displacement vector **t** – as introduced in Note (8) of Section 3.3.2.4 – does not apply here. The existence of the coincidence subset of a twin results from the *crystallographic orientation relation* (Section 3.3.2.2), which is a prerequisite for twinning. This subset is one-, two- or three-dimensional (monoperiodic, diperiodic or triperiodic) twins.

If a coincidence relation exists between lattices in direct space, a complementary superposition relation occurs for their reciprocal lattices. This superposition can often, but not always, be detected in the diffraction patterns of twinned crystals.

3.3.8.2. *Lattice coincidences, twin lattice, twin lattice index*

Four types of (exact) *lattice coincidences* have to be distinguished in twinning:

(i) *No coincidence* of lattice points (except, of course, for the initial pair). This case corresponds to arbitrary intergrowth of two crystals or to a general bicrystal.

(ii) *One-dimensional coincidence*: Both lattices have only *one lattice row* in common. Of the seven binary twin operations listed in Section 3.3.2.3.1, the following three generate one-dimensional lattice coincidence:

(*a*) twofold rotation around a (rational) lattice row [twin operation (iii) in Section 3.3.2.3.1];

(*b*) reflection across an irrational plane normal to a (rational) lattice row (note that the coincidence would be three-dimensional if this plane were rational) [twin operation (iv)];

(*c*) twofold rotation around an irrational axis normal to a (rational) lattice row (complex twin, *Kantennormalengesetz*) [twin operations (v) and (vi)].

Lattices are always centrosymmetric; hence, for lattices, as well as for centrosymmetric crystals, the first two twin operations above belong to the same twin law. For noncentrosymmetric crystals, however, the two twin operations define different twin laws.

(iii) *Two-dimensional coincidence*: Both lattices have only *one lattice plane* in common. The following two (of the seven) twin operations lead to two-dimensional lattice coincidence:

(*a*) reflection across a (rational) lattice plane [twin operation (i)];

(*b*) twofold rotation around an irrational axis normal to a (rational) lattice plane (note that the coincidence would be three-dimensional if this axis were rational) [twin operation (ii)].

Again, for lattices and centrosymmetric crystals both twin operations belong to the same twin law.

(iv) *Three-dimensional coincidence*: Here the coincidence subset is a three-dimensional lattice, the *coincidence-site lattice* or *twin lattice*. It is the three-dimensional sublattice common to the (equally or differently) oriented lattices of the two twin partners. The degree of three-dimensional lattice coincidence is defined by the *coincidence-site lattice index*, *twin lattice index* or *sublattice index* [*j*], for short: *lattice index*. This index is often called Σ, especially in metallurgy. It is the volume ratio of the primitive cells of the twin lattice and of the (original) crystal lattice (*i.e.* $1/j$ is the 'degree of dilution' of the twin lattice with respect to the crystal lattice):

$$[j] = \Sigma = V_{\rm twin}/V_{\rm crystal}.$$

The lattice index is always an integer: $j = 1$ means *complete* coincidence (parallelism), $j > 1$ *partial* coincidence of the two lattices. The index [*j*] can also be interpreted as elimination of the fraction $(j-1)/j$ of the lattice points, or as index of the translation group of the twin lattice in the translation group of the crystal lattice. The coincidence lattice, thus, is the intersection of the oriented lattices of the two twin partners.

Twinning with $[j] = 1$ has been called by Friedel (1926, p. 427) *twinning by merohedry* ('*macles par mériédrie*') (for short: *merohedral twinning*), whereas twinning with $[j] > 1$ is called *twinning by lattice merohedry* or *twinning by reticular merohedry* ('*macles par mériédrie réticulaire*') (Friedel, 1926, p. 444). The terms for $[j] = 1$ are easily comprehensible and in common use. The terms for $[j] > 1$, however, are somewhat ambiguous. In the present section, therefore, the terms *sublattice*, *coincidence lattice* or *twin lattice* of index [*j*] are preferred. Merohedral twinning is treated in detail in Section 3.3.9.

Complete and exact three-dimensional lattice coincidence ($[j] = 1$) always exists for inversion twins (of noncentrosymmetric crystals) [twin operation (vii)]. For reflection twins, complete or partial coincidence occurs if a (rational) lattice row [*uvw*] is (exactly) perpendicular to the (rational) twin reflection plane (*hkl*); similarly for rotation twins if a (rational) lattice plane (*hkl*) is (exactly) perpendicular to the (rational) twofold twin axis [*uvw*].

The systematic perpendicularity relations (*i.e.* relations valid independent of the axial ratios) for lattice planes (*hkl*) and lattice rows [*uvw*] in the various crystal systems are collected in Table 3.3.8.1. No perpendicularity occurs for triclinic lattices (except for metrical accidents). The perpendicularity cases for monoclinic and orthorhombic lattices are trivial. For tetragonal (tet), hexagonal (hex) and rhombohedral (rhomb) lattices, systematic perpendicularity of planes and rows occurs only for the $[001]_{\rm tet}$ and the $[001]_{\rm hex}$ (or $[111]_{\rm rhomb}$) zones, *i.e.* for planes parallel and rows perpendicular to these directions, in addition to the trivial cases $[001] \perp (001)$ or $[111] \perp (111)$. In cubic lattices, every lattice plane (*hkl*) is perpendicular to a lattice row [*uvw*] (with $h = u$, $k = v$, $l = w$). More general coincidence relations were derived by Grimmer (1989, 2003).

The index [*j*] of a coincidence or twin lattice can often be obtained by inspection; it can be calculated by using a formula for the auxiliary quantity j' as follows:

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