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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

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
$i = |j| = 3$.

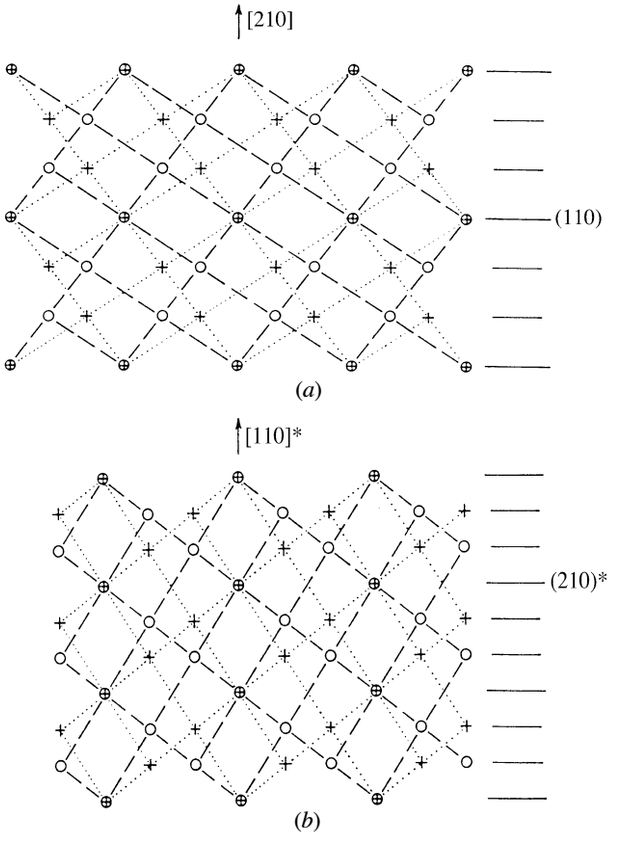

Fig. 1.3.2.1. (*a*) Projection of the lattices of the twin components of a monoclinic twinned crystal (unique axis **c**, $\gamma = 93°$) with twin index 3. The twin may be interpreted either as a rotation twin with twin axis [210] or as a reflection twin with twin plane (110). (*b*) Projection of the 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
$i = |j|/2 = 1$.

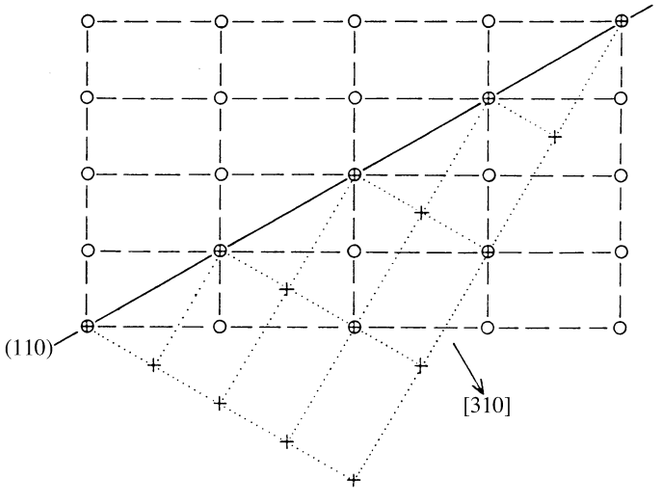

Fig. 1.3.2.2. Projection of the lattices of the twin components of an orthorhombic twinned crystal ($oP, b = \sqrt{3}a$) with twin index 2. The twin may be interpreted either as a rotation twin with twin axis [310] or as a reflection twin with twin plane (110). The figure shows, in addition, that twin 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
$i = |j|/2 = 4$.

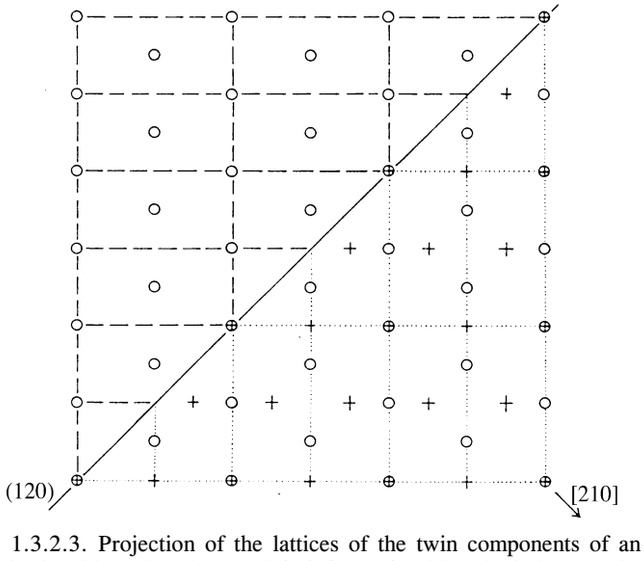

Fig. 1.3.2.3. Projection of the lattices of the twin components of an orthorhombic twinned crystal ($oC, b = 2a$) with twin index 4. The twin may be interpreted either as a rotation twin with twin axis [210] or as a reflection twin with twin plane (120).

(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

Table 1.3.4.1. *Possible twin operations for twins by merohedry*

m is the index of the point group in the corresponding holohedry; point groups allowing twins of type 2 are marked by an asterisk.

Holohedry	Bravais lattice	Point group	m	Possible twin operations
1	aP	1	2	$\bar{1}$
$2/m$	mP, mS	2 m	2 2	$\bar{1}$ $\bar{1}$
mmm	oP, oS, oI, oF	222 $mm2$	2 2	$\bar{1}$ $\bar{1}$
$4/mmm$	tP, tI	*4 *$\bar{4}$ *$4/m$ 422 $4mm$ $\bar{4}2m/\bar{4}m2$	4 4 2 2 2 2	$\bar{1}$, $.m.$, $.2.$ $\bar{1}$, $.m.$, $.2.$ $.m.$ $\bar{1}$ $\bar{1}$ $\bar{1}$
$\bar{3}m$	hR	*3 *$\bar{3}$ 32 $3m$	4 2 2 2	$\bar{1}$, $.m$, $.2$ $.m$ $\bar{1}$ $\bar{1}$
$6/mmm$	hP	*3 *$\bar{3}$ *$321/312$ *$3m1/31m$ *$\bar{3}m1/\bar{3}1m$ *6 *$\bar{6}$ *$6/m$ 622 $6mm$ $\bar{6}2m/\bar{6}m2$	8 4 4 4 2 4 4 2 2 2 2	$\bar{1}$, $.m.$, $.2.$, $m..$, $..m$, $2..$, $..2$ $.m.$, $m..$, $..m$ $\bar{1}$, $m..$, $..2/.2.$ $\bar{1}$, $m..$, $..m/.m.$ $m..$ $\bar{1}$, $.m.$, $.2.$ $\bar{1}$, $.m.$, $..m$ $.m.$ $\bar{1}$ $\bar{1}$ $\bar{1}$
$m\bar{3}m$	cP, cI, cF	*23 *$m\bar{3}$ 432 $\bar{4}3m$	4 2 2 2	$\bar{1}$, $..m$, $..2$ $..m$ $\bar{1}$ $\bar{1}$

holohedry. Column 5 shows $m-1$ possible twin operations referring to the different twin components. These twin operations are not uniquely defined (except for point group 1), but may be chosen arbitrarily from the corresponding right coset of the crystal point group in its holohedry. It is always possible, however, to choose an inversion, a reflection, or a twofold rotation as twin operation.

A twin that is not a twin by merohedry as defined above but, because of metrical specialization, has a twin lattice with twin index 1 is called a *twin by pseudo-merohedry*.

Two kinds of twins by merohedry may be distinguished.

Type 1: The twin can be described as an inversion twin. Then, only two twin components exist and the twin operation belongs to the Laue class of the crystal. As a consequence, the reciprocal lattices of the twin components are superimposed so that coinciding lattice points refer to Bragg reflections with the same $|F|^2$ values as long as Friedel's law is valid. In that case, no differences with respect to symmetry, or to reflection conditions, or to relative intensities occur between two sets of Bragg

Table 1.3.4.2. *Simulated Laue classes, extinction symbols, simulated 'possible space groups', and possible true space groups for crystals twinned by merohedry (type 2)*

Twinned crystal			Single crystal
Simulated Laue class	Twin extinction symbol	Simulated 'possible space groups'	Possible true space groups
$4/mmm$	P---	$P422$, $P4mm$, $P\bar{4}2m$, $P\bar{4}m2$, $P4/mmm$	$P4$, $P\bar{4}$, $P4/m$
	$P4_2$--	$P4_222$	$P4_2$, $P4_2/m$
	$P4_1$--	$P4_122$, $P4_322$	$P4_1$, $P4_3$
	Pn--	$P4/nmm$	$P4/n$
	$P4_2/n$--	–	$P4_2/n$
	I---	$I422$, $I4mm$, $I\bar{4}2m$, $I\bar{4}m2$, $I4/mmm$	$I4$, $I\bar{4}$, $I4/m$
	$I4_1$--	$I4_122$	$I4_1$
	$I4_1/a$--	–	$I4_1/a$
$\bar{3}m1$	P---	$P321$, $P3m1$, $P\bar{3}m1$	$P3$, $P\bar{3}$
	$P3_1$--	$P3_121$, $P3_221$	$P3_1$, $P3_2$
$\bar{3}1m$	P---	$P312$, $P31m$, $P\bar{3}1m$	$P3$, $P\bar{3}$
	$P3_1$--	$P3_112$, $P3_212$	$P3_1$, $P3_2$
$\bar{3}m$	R--	$R32$, $R3m$, $R\bar{3}m$	$R3$, $R\bar{3}$
$6/m$	P---	$P6$, $P\bar{6}$, $P6/m$	$P3$, $P\bar{3}$
	$P6_2$--	$P6_2$, $P6_4$	$P3_1$, $P3_2$
$6/mmm$	P---	$P622$, $P6mm$, $P\bar{6}m2$, $P\bar{6}2m$, $P6/mmm$	$P3$, $P\bar{3}$, $P321$, $P312$, $P3m1$, $P31m$, $P\bar{3}m1$, $P\bar{3}1m$, $P6$, $P\bar{6}$, $P6/m$
	$P6_3$--	$P6_322$	$P6_3$, $P6_3/m$
	$P6_2$--	$P6_222$, $P6_422$	$P3_1$, $P3_2$, $P3_121$, $P3_221$, $P3_112$, $P3_212$, $P6_2$, $P6_4$
	$P6_1$--	$P6_122$, $P6_522$	$P6_1$, $P6_5$
	P--c	$P6_3mc$, $P\bar{6}2c$, $P6_3/mmc$	$P31c$, $P\bar{3}1c$
	P-c-	$P6_3cm$, $P\bar{6}c2$, $P6_3/mcm$	$P3c1$, $P\bar{3}c1$
$m\bar{3}m$	P---	$P432$, $P\bar{4}3m$, $Pm\bar{3}m$	$P23$, $Pm\bar{3}$
	$P4_2$--	$P4_232$	$P2_13$
	Pn--	$Pn\bar{3}m$	$Pn\bar{3}$
	I---	$I432$, $I\bar{4}3m$, $Im\bar{3}m$	$I23$, $I2_13$, $Im\bar{3}$
	Ia--	–	$Ia\bar{3}$
	F---	$F432$, $F\bar{4}3m$, $Fm\bar{3}m$	$F23$, $Fm\bar{3}$
	Fd--	$Fd\bar{3}m$	$Fd\bar{3}$
	$P2_1/a$, b--	–	$Pa\bar{3}$

intensities measured from a single crystal on the one hand and from a twin on the other hand (whether or not the twin components differ in their volumes). If anomalous scattering is observed *and* the twin components differ in size, the intensities of Bragg reflections are changed in comparison with the untwinned crystal but the symmetry of the diffraction pattern is unchanged. For equal volumes of the twin components, however, the diffraction pattern is centrosymmetric again. The occurrence of anomalous scattering does not produce additional difficulties for space-group determination. The change of the

Bragg intensities in comparison with the untwinned crystals, however, makes a structure determination more difficult.

Type 2: The twin operation does not belong to the Laue class of the crystal. Such twins can occur only in point groups marked by an asterisk in Table 1.3.4.1, *i.e.* in 55 out of the 159 types of space groups mentioned above. If the different twin components occur with equal volumes, the corresponding diffraction pattern shows enhanced symmetry. On the contrary, the reflection conditions are unchanged in comparison to those for a single crystal, except for $Pa\bar{3}$. As a consequence, for 51 out of the 55 space-group types, the derivation of 'possible space groups', as described in *IT* A (1983, Part 3), gives incorrect results. For $P4_2/n$, $I4_1/a$ and $Ia\bar{3}$, the combination of the simulated Laue class of the twin and the (unchanged) extinction symbol does not occur for single crystals. Therefore, the symmetry of these twins can be determined uniquely. In the case of $Pa\bar{3}$, the reflection conditions differ for the two twin components. [This is because the holohedry of $Pa\bar{3}$ is $m\bar{3}m$ whereas the Laue class of the Euclidean normalizer $Ia\bar{3}$ of $Pa\bar{3}$ is $m\bar{3}$; *cf.* *IT* A (1987, Part 15).] As a consequence, the reflection conditions for such a twinned crystal differ from all conditions that may be observed for single crystals (*hkl* cyclically permutable: $0kl$ only with $k = 2n$ *or* $l = 2n$; $00l$ only with $l = 2n$) and, therefore, the true symmetry can be identified without uncertainty.

In Table 1.3.4.2, all simulated Laue classes (column 1) are listed that may be observed for twins by merohedry of type 2. Column 2 shows the corresponding extinction symbols. The symbols of the simulated 'possible space groups' that follow from *IT* A (1983, Part 3) are gathered in column 3. The last column displays the symbols of those space groups which may be the true symmetry groups for twins by merohedry showing such diffraction patterns.

1.3.5. Calculation of the twin element

If the twin element cannot be recognized by direct macroscopic or microscopic inspection, it may be calculated as described below. Given are two analogous bases **a**, **b**, **c** and **a**′, **b**′, **c**′ referring to the two twin components. If possible, both basis systems should be chosen with the same handedness. If no such bases exist, the twin is a reflection twin and one of the bases has to be replaced by its centrosymmetrical one, *e.g.* **a**′, **b**′, **c**′ by $-\mathbf{a}'$, $-\mathbf{b}'$, $-\mathbf{c}'$. The relation between the two bases is described by

$$\mathbf{a}' = e_{11}\mathbf{a} + e_{12}\mathbf{b} + e_{13}\mathbf{c},$$
$$\mathbf{b}' = e_{21}\mathbf{a} + e_{22}\mathbf{b} + e_{23}\mathbf{c},$$
$$\mathbf{c}' = e_{31}\mathbf{a} + e_{32}\mathbf{b} + e_{33}\mathbf{c}.$$

The coefficients e_{ij} have to be obtained by measurement.

Basis **a**, **b**, **c** may be mapped onto **a**′, **b**′, **c**′ by a pure rotation that brings **a** to **a**′, **b** to **b**′, and **c** to **c**′. To derive the direction of the rotation axis, calculate the three vectors

$$\mathbf{a}_1 = \mathbf{a} + \mathbf{a}', \quad \mathbf{b}_1 = \mathbf{b} + \mathbf{b}', \quad \mathbf{c}_1 = \mathbf{c} + \mathbf{c}'.$$

$\mathbf{a}_1$, $\mathbf{b}_1$, $\mathbf{c}_1$ bisect the angles $\sigma_a = \mathbf{a} \wedge \mathbf{a}'$, $\sigma_b = \mathbf{b} \wedge \mathbf{b}'$, and $\sigma_c = \mathbf{c} \wedge \mathbf{c}'$, respectively. Calculate three further vectors of arbitrary length $\mathbf{a}_2, \mathbf{b}_2, \mathbf{c}_2$ which are perpendicular to the planes defined by **a** and **a**′, **b** and **b**′, and **c** and **c**′, respectively, from the scalar products

$$\mathbf{a}_2 \cdot \mathbf{a} = \mathbf{a}_2 \cdot \mathbf{a}' = 0,$$
$$\mathbf{b}_2 \cdot \mathbf{b} = \mathbf{b}_2 \cdot \mathbf{b}' = 0,$$
$$\mathbf{c}_2 \cdot \mathbf{c} = \mathbf{c}_2 \cdot \mathbf{c}' = 0.$$

The plane defined by $\mathbf{a}_1$ and $\mathbf{a}_2$ is perpendicular to the plane defined by **a** and **a**′ and bisects the angle $\mathbf{a} \wedge \mathbf{a}'$. Analogous planes refer to $\mathbf{b}_1$ and $\mathbf{b}_2$, and $\mathbf{c}_1$ and $\mathbf{c}_2$. Vectors $\mathbf{r}_a$, $\mathbf{r}_b$, and $\mathbf{r}_c$ lying within one of these planes may be described as linear combinations of $\mathbf{a}_1$ and $\mathbf{a}_2$, $\mathbf{b}_1$and $\mathbf{b}_2$, or $\mathbf{c}_1$ and $\mathbf{c}_2$, respectively:

$$\mathbf{r}_a = \lambda_a\mathbf{a}_1 + \mu_a\mathbf{a}_2,$$
$$\mathbf{r}_b = \lambda_b\mathbf{b}_1 + \mu_b\mathbf{b}_2,$$
$$\mathbf{r}_c = \lambda_c\mathbf{c}_1 + \mu_c\mathbf{c}_2.$$

The common intersection line of these three planes is parallel to the twin axis. It may be calculated by solving any of the three equations

$$\mathbf{r}_a = \mathbf{r}_b, \quad \mathbf{r}_a = \mathbf{r}_c, \quad \text{or} \quad \mathbf{r}_b = \mathbf{r}_c.$$

$\mathbf{r}_a = \mathbf{r}_b$: choose λ_a arbitrarily equal to 1.

$$\mathbf{a}_1 + \mu_a\mathbf{a}_2 = \lambda_b\mathbf{b}_1 + \mu_b\mathbf{b}_2.$$

Solve the inhomogeneous system of three equations that corresponds to this vector equation for the three variables μ_a, λ_b, and μ_b. Calculate the vector $\mathbf{r} = \mathbf{a}_1 + \mu_a\mathbf{a}_2$. Its components with respect to **a**, **b**, **c** describe the direction of the twin axis.

The angle τ of the twin rotation may then be calculated by

$$\sin\tfrac{1}{2}\tau = \frac{\sin\frac{1}{2}\sigma_a}{\sin\delta_a} = \frac{\sin\frac{1}{2}\sigma_b}{\sin\delta_b} = \frac{\sin\frac{1}{2}\sigma_c}{\sin\delta_c}$$

with $\delta_a = \mathbf{r} \wedge \mathbf{a}$, $\delta_b = \mathbf{r} \wedge \mathbf{b}$, $\delta_c = \mathbf{r} \wedge \mathbf{c}$.

If the basis **a**, **b**, **c** is orthogonal, τ may be obtained from

$$\cos\tau = \tfrac{1}{2}(\cos\sigma_a + \cos\sigma_b + \cos\sigma_c - 1).$$

If the coefficients of **r** are rational and τ equals 180°, then **r** describes the direction either of the twofold twin axis or of the normal of the twin plane. If **r** is rational and τ equals 60, 90 or 120°, **r** is parallel to the twin axis. If **r** is irrational, but τ equals 180° and there exists, in addition, a net plane perpendicular to **r**, this net plane describes the twin plane.

If none of these conditions is fulfilled, one has to repeat the calculations with a differently chosen basis system for one of the twin components. The number of possibilities for this choice depends on the lattice symmetry. The following list gives all equivalent basis systems for all descriptions of Bravais lattices used in *IT* A (1983):

aP: $\mathbf{a}, \mathbf{b}, \mathbf{c}$;

mP, *mS* (unique axis **b**): $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $-\mathbf{a}, \mathbf{b}, -\mathbf{c}$;

mP, *mS* (unique axis **c**): $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $-\mathbf{a}, -\mathbf{b}, \mathbf{c}$;

oP, *oS*, *oI*, *oF*: $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $-\mathbf{a}, -\mathbf{b}, \mathbf{c}$; $-\mathbf{a}, \mathbf{b}, -\mathbf{c}$; $\mathbf{a}, -\mathbf{b}, -\mathbf{c}$;

tP, *tI*: $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $-\mathbf{a}, -\mathbf{b}, \mathbf{c}$; $-\mathbf{a}, \mathbf{b}, -\mathbf{c}$; $\mathbf{a}, -\mathbf{b}, -\mathbf{c}$;
$\mathbf{b}, -\mathbf{a}, \mathbf{c}$; $-\mathbf{b}, \mathbf{a}, \mathbf{c}$; $\mathbf{b}, \mathbf{a}, -\mathbf{c}$; $-\mathbf{b}, -\mathbf{a}, -\mathbf{c}$;

hP: $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $\mathbf{b}, -\mathbf{a}-\mathbf{b}, \mathbf{c}$; $-\mathbf{a}-\mathbf{b}, \mathbf{a}, \mathbf{c}$; $\mathbf{b}, \mathbf{a}, -\mathbf{c}$;
$-\mathbf{a}-\mathbf{b}, \mathbf{b}, -\mathbf{c}$; $\mathbf{a}, -\mathbf{a}-\mathbf{b}, -\mathbf{c}$; $-\mathbf{a}, -\mathbf{b}, \mathbf{c}$; $-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$;
$\mathbf{a}+\mathbf{b}, -\mathbf{a}, \mathbf{c}$; $-\mathbf{b}, -\mathbf{a}, -\mathbf{c}$; $\mathbf{a}+\mathbf{b}, -\mathbf{b}, -\mathbf{c}$; $-\mathbf{a}, \mathbf{a}+\mathbf{b}, -\mathbf{c}$;

hR (hexagonal description): $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $\mathbf{b}, -\mathbf{a}-\mathbf{b}, \mathbf{c}$;
$-\mathbf{a}-\mathbf{b}, \mathbf{a}, \mathbf{c}$; $\mathbf{b}, \mathbf{a}, -\mathbf{c}$; $-\mathbf{a}-\mathbf{b}, \mathbf{b}, -\mathbf{c}$; $\mathbf{a}, -\mathbf{a}-\mathbf{b}, -\mathbf{c}$;

hR (rhombohedral description): $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $\mathbf{b}, \mathbf{c}, \mathbf{a}$; $\mathbf{c}, \mathbf{a}, \mathbf{b}$;
$-\mathbf{b}, -\mathbf{a}, -\mathbf{c}$; $-\mathbf{a}, -\mathbf{c}, -\mathbf{b}$; $-\mathbf{c}, -\mathbf{b}, -\mathbf{a}$;

cP, *cI*, *cF*: $\mathbf{a}, \mathbf{b}, \mathbf{c}$; $\mathbf{b}, \mathbf{c}, \mathbf{a}$; $\mathbf{c}, \mathbf{a}, \mathbf{b}$; $-\mathbf{a}, -\mathbf{b}, \mathbf{c}$;
$-\mathbf{b}, \mathbf{c}, -\mathbf{a}$; $\mathbf{c}, -\mathbf{a}, -\mathbf{b}$; $-\mathbf{a}, \mathbf{b}, -\mathbf{c}$; $\mathbf{b}, -\mathbf{c}, -\mathbf{a}$;
$-\mathbf{c}, -\mathbf{a}, \mathbf{b}$; $\mathbf{a}, -\mathbf{b}, -\mathbf{c}$; $-\mathbf{b}, -\mathbf{c}, \mathbf{a}$; $-\mathbf{c}, \mathbf{a}, -\mathbf{b}$;
$-\mathbf{b}, -\mathbf{a}, -\mathbf{c}$; $-\mathbf{a}, -\mathbf{c}, -\mathbf{b}$; $-\mathbf{c}, -\mathbf{b}, -\mathbf{a}$; $\mathbf{b}, \mathbf{a}, -\mathbf{c}$;
$\mathbf{a}, -\mathbf{c}, \mathbf{b}$; $-\mathbf{c}, \mathbf{b}, \mathbf{a}$; $\mathbf{b}, -\mathbf{a}, \mathbf{c}$; $-\mathbf{a}, \mathbf{c}, \mathbf{b}$; $\mathbf{c}, \mathbf{b}, -\mathbf{a}$;
$-\mathbf{b}, \mathbf{a}, \mathbf{c}$; $\mathbf{a}, \mathbf{c}, -\mathbf{b}$; $\mathbf{c}, -\mathbf{b}, \mathbf{a}$.

1.4.2.1. *Symmorphic space groups*

The 73 space groups known as 'symmorphic' are in one-to-one correspondence with the arithmetic crystal classes, and their standard 'short' symbols (Bertaut, 1995) are obtained by interchanging the order of the geometric crystal class and the Bravais cell in the symbol for the arithmetic space group. In fact, conventional crystallographic symbolism did not distinguish between arithmetic crystal classes and symmorphic space groups until recently (de Wolff *et al.*, 1985); the symbol of the symmorphic group was used also for the arithmetic class.

This relationship between the symbols, and the equivalent rule-of-thumb *symmorphic space groups are those whose standard (short) symbols do not contain glide planes or screw axes*, reveal nothing fundamental about the nature of symmorphism; they are simply a consequence of the conventions governing the construction of symbols in *International Tables for Crystallography*.*

Although the *standard* symbols of the symmorphic space groups do not contain screw axes or glide planes, this is a result of the manner in which the space-group symbols have been devised. Most symmorphic space groups do in fact contain screw axes and/or glide planes. This is immediately obvious for the symmorphic space groups based on centred cells; *C*2 contains equal numbers of diad rotation axes and diad screw axes, and *Cm* contains equal numbers of reflection planes and glide planes. This is recognized in the 'extended' space-group symbols (Bertaut, 1995), but these are clumsy and not commonly used; those for *C*2 and *Cm* are $C1^{2}_{2_1}1$ and $C1^{m}_{a}1$, respectively. In the more symmetric crystal systems, even symmorphic space groups with primitive cells contain screw axes and/or glide planes; *P*422 ($P42^{2}_{2_1}$) contains many diad screw axes and *P*4/*mmm* ($P4/m2/m^{2/m}_{2_1/g}$) contains both screw axes and glide planes.

The balance of symmetry elements within the symmorphic space groups is discussed in more detail in Subsection 9.7.1.2.

1.4.3. Effect of dispersion on diffraction symmetry

In the absence of dispersion ('anomalous scattering'), the intensities of the reflections *hkl* and $\bar{h}\bar{k}\bar{l}$ are equal (Friedel's law), and statements about the symmetry of the weighted reciprocal lattice and quantities derived from it often rest on the tacit or explicit assumption of this law – the condition underlying it being forgotten. In particular, if dispersion is appreciable, the symmetry of the Patterson synthesis and the 'Laue' symmetry are altered.

1.4.3.1. *Symmetry of the Patterson function*

In Volume A of *International Tables*, the symmetry of the Patterson synthesis is derived in two stages. First, any glide planes and screw axes are replaced by mirror planes and the corresponding rotation axes, giving a symmorphic space group (Subsection 1.4.2.1). Second, a centre of symmetry is added. This second step involves the tacit assumption of Friedel's law, and should not be taken if any atomic scattering factors have appreciable imaginary components. In such cases, the symmetry of the Patterson synthesis will not be that of one of the 24 centrosymmetric symmorphic space groups, as given in Volume A, but will be that of the symmorphic space group belonging to the arithmetic crystal class to which the space group of the structure belongs. There are thus 73 possible Patterson symmetries.

An equivalent description of such symmetries, in terms of 73 of the 1651 dichromatic colour groups, has been given by Fischer & Knop (1987); see also Wilson (1993).

1.4.3.2. *'Laue' symmetry*

Similarly, the eleven conventional 'Laue' symmetries [*International Tables for Crystallography* (1995), Volume A, p. 40 and elsewhere] involve the explicit assumption of Friedel's law. If dispersion is appreciable, the 'Laue' symmetry may be that of any of the 32 point groups. The point group, in correct orientation, is obtained by dropping the Bravais-lattice symbol from the symbol of the arithmetic crystal class or of the Patterson symmetry.

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* Three examples of informative definitions are:

1. The space group corresponding to the zero solution of the Frobenius congruences is called a symmorphic space group (Engel, 1986, p. 155).

2. A space group *F* is called *symmorphic* if one of its finite subgroups (and therefore an infinity of them) is of an order equal to the order of the point group R_r (Opechowski, 1986, p. 255).

3. A space group is called *symmorphic* if the coset representatives W_j can be chosen in such a way that they leave one common point fixed (Wondratschek, 1995, p. 717).

Even in context, these are pretty opaque.

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