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