3. PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

interest is a different optical birefringence in different growth sectors (optical anomaly) because this may simulate twinning. A typical example of this optical anomaly is shown in Fig. 3.3.1.2.

The phenomenon *optical anomaly* can be explained as follows: as a rule, impurities (or dopants) present in the solution are incorporated into the crystal during growth. Usually, the impurity concentrations differ in symmetrically *non-equivalent* growth sectors (which belong to different crystal forms), leading to slightly changed lattice parameters and physical properties of these sectors. Surprisingly, optical anomalies may occur also in symmetrically *equivalent* growth sectors (which belong to the same crystal form): as a consequence of growth fluctuations, layers of varying impurity concentrations parallel to the growth face of the sector ('growth striations') are formed. This causes a slight change of the interplanar spacing normal to the growth face. For example, a cubic NaCl crystal grown on {100} cube faces from an aqueous solution containing Mn ions consists of three pairs of (opposite) growth sectors exhibiting a slight tetragonal distortion with tetragonality 10^{-5} along their $\langle 100 \rangle$ growth directions, and, hence, are optically uniaxial (Ikeno *et al.*, 1968). Although this phenomenon closely resembles all features of twinning, it does not belong to the category 'twinning', because it is not an intrinsic property of the crystal species, but rather the result of different growth conditions (or growth mechanisms) on different faces of the same crystal (growth anisotropy).

An analogous effect may be observed in crystals grown from the melt on rounded and facetted interfaces (*e.g.* garnets). The regions crystallized on the rounded growth faces and on the different facets correspond to different growth sectors and may exhibit optical anomalies.

The relative lattice-parameter changes associated with these phenomena usually are smaller than 10^{-4} and cannot be detected in ordinary X-ray diffraction experiments. They are, however, accessible by high-resolution X-ray diffraction.

(v) *Translation domains*: Translation domains are homogeneous crystal regions that exhibit exact parallel orientations, but are displaced with respect to each other by a vector (frequently called a *fault vector*), which is a fraction of a lattice translation vector. The interface between adjoining translation domains is called the 'translation boundary'. Often the terms *antiphase domains* and *antiphase boundaries* are used. Special cases of translation boundaries are stacking faults. Translation domains are defined on an atomic scale, whereas the term parallel intergrowth [see item (ii) above] refers to macroscopic (morphological) phenomena; *cf.* Note (7) in Section 3.3.2.4.

(vi) *Twins*: A frequently occurring intergrowth of two or more crystals of the same species with well defined *crystallographic* orientation relations is called a *twin* (German: *Zwilling*; French: *macle*). Twins form the subject of the present chapter. The closely related topic of *domain structures* is treated in Chapter 3.4.

3.3.2. Basic concepts and definitions of twinning

Because twinning is a rather complex and widespread phenomenon, several definitions have been presented in the literature. Two of them are quoted here because of the particular engagement of their authors in this topic.

George Friedel (1904; 1926, p. 421): *A twin is a complex crystalline edifice built up of two or more homogeneous portions of the same crystal species in contact (juxtaposition) and oriented with respect to each other according to well-defined laws.*

These laws, as formulated by Friedel, are specified in his book (Friedel, 1926). His 'lattice theory of twinning' is discussed in Sections 3.3.8 and 3.3.9 of the present chapter.

Paul Niggli (1919, 1920/1924/1941): *If several crystal individuals of the same species are intergrown in such a way that all analogous faces and edges are parallel, then one speaks of parallel intergrowth. If for two crystal individuals not all but only some of the (morphological) elements (edges or faces), at least two independent ones, are parallel or antiparallel, and if such an intergrowth due to its frequent occurrence is not 'accidental', then one speaks of twins or twin formation. The individual partners of typical twins are either mirror images with respect to a common plane ('twin-plane law'), or they appear rotated by 180° around a (common) direction ('zone-axis law', 'hemitropic twins'), or both features occur together. These planes or axes, or both, for all frequently occurring twins turn out to be elements with relatively simple indices (referred to the growth morphology).* (Niggli, 1924, p. 176; 1941, p. 137.)

Both definitions are geometric. They agree in the essential fact that the 'well defined' laws, *i.e.* the orientation relations between two twin partners, refer to rational planes and directions. Morphologically, these relations find their expression in the parallelism of some crystal edges and crystal faces. In these and other classical definitions of twins, the structure and energy of twin boundaries were not included. This aspect was first introduced by Buerger in 1945.

3.3.2.1. *Definition of a twin*

In a more extended fashion we define twinning as follows:

An intergrowth of two or more macroscopic, congruent or enantiomorphic, individuals of the same crystal species is called a *twin*, if the orientation relations between the individuals occur frequently and are 'crystallographic'. The individuals are called twin components, twin partners or twin domains. A twin is characterized by the *twin law*, *i.e.* by the *orientation and chirality relation* of two twin partners, as well as by their *contact relation* (twin interface, composition plane, domain boundary).

3.3.2.2. *Essential addenda to the definition*

(*a*) The orientation relation between two partners is defined as *crystallographic* and, hence, the corresponding intergrowth is a *twin*, if the following two minimal conditions are *simultaneously* obeyed:

(i) at least *one* lattice row (crystal edge) $[uvw]$ is '*common*' to both partners I and II, either parallel or antiparallel, *i.e.* $[uvw]_\text{I}$ is parallel to $\pm[uvw]_\text{II}$;

(ii) at least *two* lattice planes (crystal faces) $(hkl)_\text{I}$ and $\pm(hkl)_\text{II}$, one from each partner, are '*parallel*', but not necessarily '*common*' (see below). This condition implies a *binary twin operation* (twofold rotation, reflection, inversion).

Both conditions taken together define the *minimal* geometric requirement for a twin (at least one common row *and* one pair of parallel planes), as originally pronounced by several classical authors (Tschermak, 1884, 1905; 1904; Tschermak & Becke, 1915; Mügge, 1911, p. 39; Niggli, 1920/1924/1941; Tertsch, 1936) and taken up later by Menzer (1955) and Hartman (1956). It is obvious that these crystallographic conditions apply even more to twins with two- and three-dimensional lattice coincidences, as described in Section 3.3.8. Other orientation relations, as they occur, for instance, in arbitrary intergrowths or bicrystals, are called 'noncrystallographic'.

The terms 'common edge' and 'common face', as used in this section, are derived from the original morphological consideration of twins. Example: a re-entrant edge of a twin is common to both twin partners. In lattice considerations, the terms 'common lattice row', 'common lattice plane' and 'common lattice' require a somewhat finer definition, in view of a possible *twin displacement vector* **t** of the twin boundary, as introduced in Note (8) of

Section 3.3.2.4 and in Section 3.3.10.3. For this distinction the terms 'parallel', 'common' and 'coincident' are used as follows:

Two lattice rows $[uvw]_I$ *and* $[uvw]_{II}$:
Common: rows parallel or antiparallel, with their lattice points possibly displaced with respect to each other parallel to the row by a vector $\mathbf{t} \neq \mathbf{0}$.
Coincident: common rows with pointwise coincidence of their lattice points, *i.e.* $\mathbf{t} = \mathbf{0}$.

Two lattice planes $(hkl)_I$ *and* $(hkl)_{II}$:
Parallel: 'only' the planes as such, but *not all* corresponding lattice rows in the planes, are mutually parallel or antiparallel.
Common: parallel planes with *all* corresponding lattice rows mutually parallel or antiparallel, but possibly displaced with respect to each other parallel to the plane by a vector $\mathbf{t} \neq \mathbf{0}$.
Coincident: common planes with pointwise coincidence of their lattice points, *i.e.* $\mathbf{t} = \mathbf{0}$.

Two point lattices I and II:
Parallel or *common*: all corresponding lattice rows are mutually parallel or antiparallel, but the lattices are possibly displaced with respect to each other by a vector $\mathbf{t} \neq \mathbf{0}$.
Coincident: parallel lattices with pointwise coincidence of their lattice points, *i.e.* $\mathbf{t} = \mathbf{0}$.

Note that for lattice rows and point lattices only two cases have to be distinguished, whereas lattice planes require three terms.

(*b*) A twinned crystal may consist of more than two individuals. All individuals that have the same orientation and handedness belong to the same *orientation state* (*component state*, *domain state*, *domain variant*). The term 'twin' for a crystal aggregate requires the presence of at least two orientation states.

 (*c*) The orientation and chirality relation between two twin partners is expressed by the *twin law*. It comprises the set of *all twin operations* that transform the two orientation states into each other. A twin operation cannot be a symmetry operation of either one of the two twin components. The combination of a twin operation and the geometric element to which it is attached is called a *twin element* (*e.g.* twin mirror plane, twofold twin axis, twin inversion centre).

(*d*) An orientation relation between two individuals deserves the name '*twin law*' only if it occurs frequently, is reproducible and represents an inherent feature of the crystal species.

(*e*) One feature which facilitates the formation of twins is *pseudosymmetry*, apparent either in the crystal structure, or in special lattice-parameter ratios or lattice angles.

(*f*) In general, the twin interfaces are low-energy boundaries with good structural fit; very often they are low-index lattice planes.

3.3.2.3. *Specifications and extensions of the orientation relations*

In the following, the orientation and chirality relations of two or more twin components, only briefly mentioned in the definition, are explained in detail. Two categories of orientation relations have to be distinguished: those arising from *binary twin operations* (*binary twin elements*), *i.e.* operations of order 2, and those arising from *pseudo n-fold twin rotations* (*n-fold twin axes*), *i.e.* operations of order ≥ 3.

3.3.2.3.1. *Binary twin operations (twin elements)*

The (crystallographic) orientation relation of two twin partners can be expressed either by a *twin operation* or by its corresponding *twin element*. Binary twin elements can be either *twin mirror planes* or *twofold twin axes* or *twin inversion centres*. The former two twin elements must be parallel or normal to (possible) crystal faces and edges (macroscopic description) or, equivalently, parallel or normal to lattice planes and lattice rows (microscopic lattice description). Twin elements may be either rational (integer indices) or irrational (irrational indices which, however, can always be approximated by sufficiently large integer indices). Twin reflection planes and twin axes *parallel* to lattice planes or lattice rows are always rational. Twin axes and twin mirror planes *normal* to lattice planes or lattice rows are either rational or irrational. In addition to planes and axes, points can also occur as twin elements: *twin inversion centres*.

There exist seven kinds of binary twin elements that define the seven general twin laws possible for noncentrosymmetric triclinic crystals (crystal class 1):

(i) *Rational* twin mirror plane (hkl) normal to an irrational line: *reflection twin* (Fig. 3.3.2.1*a*). The lattice plane *hkl* is common to both twin partners.
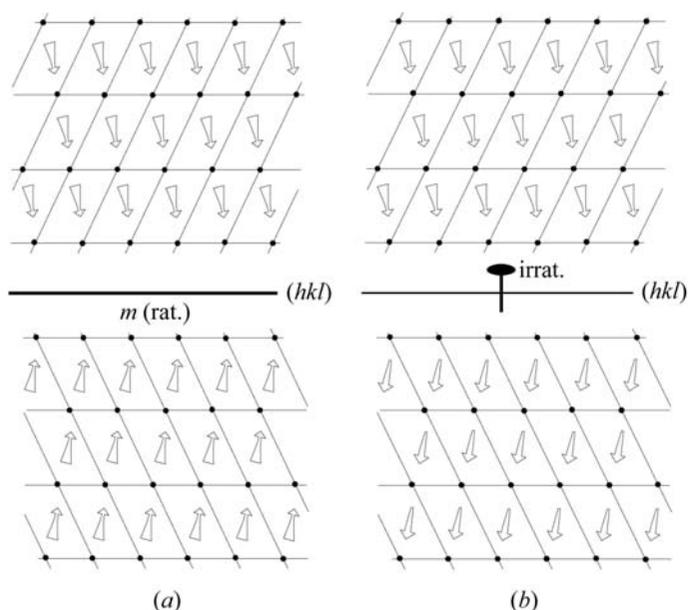

Fig. 3.3.2.1. Schematic illustration of the orientation relations of triclinic twin partners, see Section 3.3.2.3.1, (*a*) for twin element (i) 'rational twin mirror plane' and (*b*) for twin element (ii) 'irrational twofold twin axis' (see text); common lattice plane (*hkl*) for both cases. The noncentrosymmetry of the crystal is indicated by arrows. The sloping up and sloping down of the arrows is indicated by the tapering of their images. For centrosymmetry, both cases (*a*) and (*b*) represent the same orientation relation.
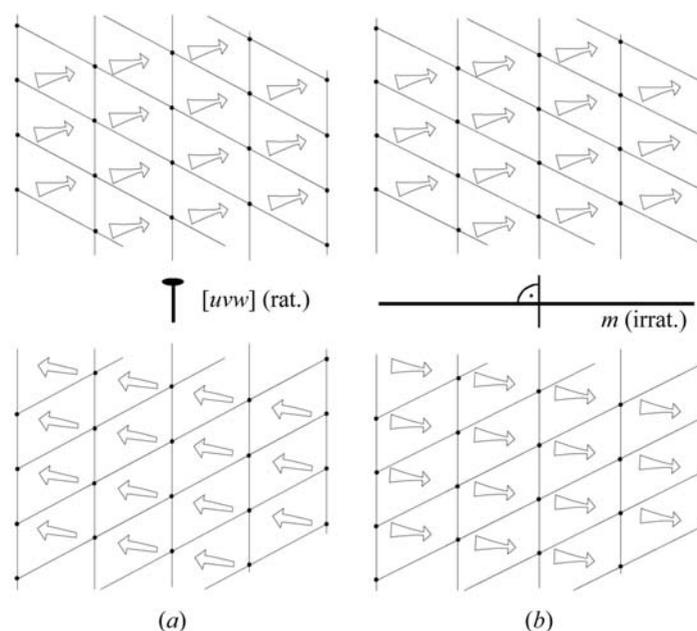

Fig. 3.3.2.2. As Fig. 3.3.2.1, (*a*) for twin element (iii) 'rational twofold twin axis' and (*b*) for twin element (iv) 'irrational twin mirror plane' (see text); common lattice row [*uvw*] for both cases. For centrosymmetry, both cases represent the same orientation relation.
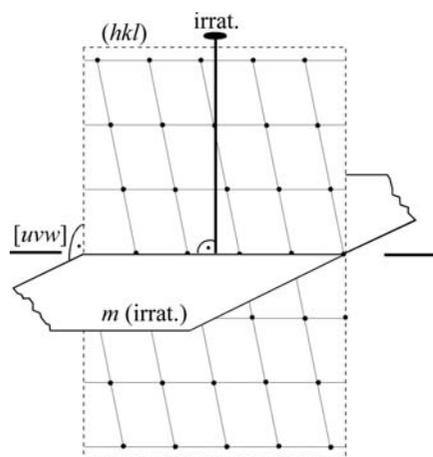
Fig. 3.3.2.3. Illustration of the *Kantennormalengesetz* (complex twin) for twin elements (v) and (vi) (see text); common lattice row [*uvw*] for both cases. Note that both twin elements transform the net plane (*hkl*)$_I$ into its parallel but not pointwise coincident counterpart (*hkl*)$_{II}$. For centrosymmetry, both cases represent the same orientation relation.

(ii) *Irrational* twofold twin axis normal to a rational lattice plane *hkl*: *rotation twin* (Fig. 3.3.2.1*b*). The lattice plane *hkl* is common to both twin partners.

(iii) *Rational* twofold twin axis [*uvw*] normal to an irrational plane: *rotation twin* (Fig. 3.3.2.2*a*). The lattice row [*uvw*] is common to both twin partners.

(iv) *Irrational* twin mirror plane normal to a rational lattice row [*uvw*]: *reflection twin* (Fig. 3.3.2.2*b*). The lattice row [*uvw*] is common to both twin partners.

(v) *Irrational* twofold twin axis normal to a rational lattice row [*uvw*], both located in a rational lattice plane (*hkl*); perpendicular to the irrational twin axis is an irrational plane: *complex twin*; German: *Kantennormalengesetz* (Fig. 3.3.2.3). The lattice row [*uvw*] is 'common' to both twin partners; the planes (*hkl*)$_I$ and (*hkl*)$_{II}$ are 'parallel' but not 'common' (*cf.* Tschermak & Becke, 1915, p. 98; Niggli, 1941, p. 138; Bloss, 1971, pp. 228–230; Phillips, 1971, p. 178).

(vi) *Irrational* twin mirror plane containing a rational lattice row [*uvw*]; perpendicular to the twin plane is an irrational direction; the row [*uvw*] and the perpendicular direction span a rational lattice plane (*hkl*): *complex twin*; this 'inverted *Kantennormalengesetz*' is not described in the literature (Fig. 3.3.2.3). The row [*uvw*] is 'common' to both twin partners; the planes (*hkl*)$_I$ and (*hkl*)$_{II}$ are 'parallel' but not 'common'.

(vii) *Twin inversion centre*: *inversion twin*. The three-dimensional lattice is common to both twin partners. Inversion twins are always merohedral (parallel-lattice) twins (*cf.* Section 3.3.8).

All these binary twin elements – no matter whether rational or irrational – lead to *crystallographic* orientation relations, as defined in Section 3.3.2.2, because the following lattice items belong to both twin partners:

(*a*) The rational lattice planes (*hkl*)$_I$ and (*hkl*)$_{II}$ are 'common' for cases (i) and (ii) (Fig. 3.3.2.1).

(*b*) The rational lattice rows [*uvw*]$_I$ and [*uvw*]$_{II}$ are 'common' and furthermore lattice planes (*hkl*)$_I$/(*hkl*)$_{II}$ in the zone [*uvw*] are 'parallel', but not 'common' for cases (iii), (iv), (v) and (vi). Note that for cases (iii) and (iv) any two planes (*hkl*)$_I$/(*hkl*)$_{II}$ of the zone [*uvw*] are parallel, whereas for cases (v) and (vi) only a single pair of parallel planes exists (*cf.* Figs. 3.3.2.2 and 3.3.2.3).

(*c*) The entire three-dimensional lattice is 'common' for case (vii).

In this context one realizes which wide range of twinning is covered by the requirement of a *crystallographic* orientation relation: the 'minimal' condition is provided by the *complex twins*

(v) and (vi): only a one-dimensional lattice row is 'common', two lattice planes are 'parallel' and all twin elements are irrational (Fig. 3.3.2.3). The 'maximal' condition, a 'common' three-dimensional lattice, occurs for *inversion twins* ('merohedral' or 'parallel-lattice twins'), case (vii).

In *noncentrosymmetric* triclinic crystals, the above twin elements define seven different twin laws, but for *centrosymmetric* crystals only three of them represent different orientation relations, because both in lattices and in centrosymmetric crystals a twin mirror plane defines the same orientation relation as the twofold twin axis normal to it, and *vice versa*. Consequently, the twin elements of the three pairs (i) + (ii), (iii) + (iv) and (v) + (vi) represent the same orientation relation. Case (vii) does not apply to centrosymmetric crystals, since here the inversion centre already belongs to the symmetry of the crystal.

For symmetries higher than triclinic, even more twin elements may define the same orientation relation, *i.e.* form the same twin law. Example: the dovetail twin of gypsum (point group 12/*m*1) with twin mirror plane (100) can be described by the four alternative twin elements (i), (ii), (iii), (iv) (*cf.* Section 3.3.4, Fig. 3.3.4.1). Furthermore, with increasing symmetry, the twin elements (i) and (iii) may become even more special, and the nature of the twin type may change as follows:

(i) the line normal to a rational twin mirror plane (*hkl*) may become a *rational* line [*uvw*];

(ii) the plane normal to a rational twofold twin axis [*uvw*] may become a *rational* plane (*hkl*).

In both cases, the three-dimensional lattice (or a sublattice of it) is now common to both twin partners, *i.e.* a 'merohedral' twin results.

There is one more binary twin type which seems to reduce even further the above-mentioned 'minimal' condition for a crystallographic orientation relation, the so-called '*median law*' (German: *Mediangesetz*) of Brögger (1890), described by Tschermak & Becke (1915, p. 99). So far, it has been found in one mineral only: hydrargillite (modern name gibbsite), Al(OH)$_3$. The acceptability of this orientation relation as a twin law is questionable; see Section 3.3.6.10.

3.3.2.3.2. *Pseudo n-fold twin rotations (twin axes) with $n \geq 3$*

There is a long-lasting controversy in the literature, *e.g.* Hartman (1956, 1960), Buerger (1960*b*), Curien (1960), about the acceptance of three-, four- and sixfold rotation axes as twin elements, for the following reason:

Twin operations of order two (reflection, twofold rotation, inversion) are 'exact', *i.e.* in a component pair they transform the orientation state of one component exactly into that of the other. There occur, in addition, many cases of multiple twins, which can be described by three-, four- and sixfold twin axes. These axes, however, are *pseudo axes* because their rotation angles are close to but not exactly equal to 120, 90 or 60°, due to metrical deviations (no matter how small) from a higher-symmetry lattice. A well known example is the triple twin (German: *Drilling*) of orthorhombic aragonite, where the rotation angle $\gamma = 2 \arctan b/a = 116.2°$ (which transforms the orientation state of one component exactly into that of the other) deviates significantly from the 120° angle of a proper threefold rotation (Fig. 3.3.2.4). Another case of $n = 3$ with a very small metrical deviation is provided by ammonium lithium sulfate ($\gamma = 119.6°$).

All these (pseudo) *n*-fold rotation twins, however, can also be described by (exact) binary twin elements, *viz* by a cyclic sequence of twin mirror planes or twofold twin axes. This is also illustrated and explained in Fig. 3.3.2.4. This possibility of describing cyclic twins by 'exact' binary twin operations is the reason why Hartman (1956, 1960) and Curien (1960) do not consider 'non-exact' three-, four- and sixfold rotations as proper twin operations.
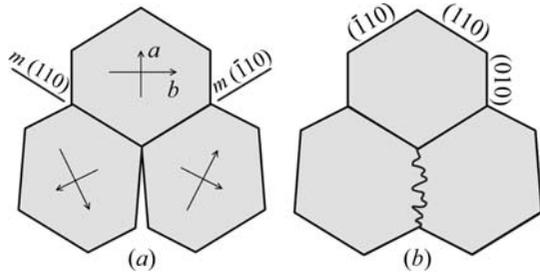
Fig. 3.3.2.4. (*a*) Triple growth twin of orthorhombic aragonite, CaCO$_3$, with pseudo-threefold twin axis. The gap angle is 11.4°. The exact description of the twin aggregate by means of two symmetrically equivalent twin mirror planes (110) and ($\bar{1}$10) is indicated. In actual crystals, the gap is usually closed as shown in (*b*).

The crystals forming twins with pseudo *n*-fold rotation axes always exhibit *metrical pseudosymmetries*. In the case of transformation twins and domain structures, the metrical pseudosymmetries of the low-symmetry (deformed) phase $\mathcal{H}$ result from the *true structural* symmetry $\mathcal{G}$ of the parent phase (*cf.* Section 3.3.7.2). This aspect caused several authors [*e.g.* Friedel, 1926, p. 435; Donnay (*cf.* Hurst *et al.*, 1956); Buerger, 1960*b*] to accept these pseudo axes for the treatment of twinning. The present authors also recommend including three-, four- and sixfold rotations as permissible twin operations. The consequences for the definition of the twin law will be discussed in Section 3.3.4 and in Section 3.4.3. For a further extension of this concept to fivefold and tenfold multiple growth twins, see Note (6) below and Example 3.3.6.8.

3.3.2.4. *Notes on the definition of twinning*

(1) The above definition of twinning covers twins with a *size range* from decimetres for large mineral specimens to fractions of microns of polydomain twins. The lower limit for a reasonable application of the twin concept lies in the nanometre range of 100–1000 Å. *Unit-cell twinning* is a limiting case closely related to superstructures or positional disorder and is not treated in this chapter. An extensive monograph on this topic under the name *Tropochemical cell-twinning* was recently published by Takeuchi (1997).

(2) *Rational twin elements* are designated by integer Miller indices (*hkl*) and integer direction indices [*uvw*] for twin mirror planes and twin rotation axes, respectively; the values of these indices usually are small numbers, < 6. Larger values should not be accepted without critical assessment. Irrational twin elements are described either by their rational 'counterparts' (perpendicular planes or lines) or are approximated by high integer values of the indices.

(3) For a twin, the *crystallographic orientation relation* is a property of the crystal structure, in contrast to bicrystals, where the given orientation relation is either accidental or enforced by the experiment. If such an orientation relation happens to be crystallographic, the bicrystal could formally be considered to be a twin. It is not recommended, however, to accept such a bicrystal as a twin because its orientation relation does not form 'spontaneously' as a property of the structure.

(4) There are some peculiarities about the *contact relations* between two twin components. Often quite different twin boundaries occur for one and the same orientation relation. The boundaries are either irregular (frequently in penetration twins) or planar interfaces. Even though crystallographic boundaries are the most frequent interfaces, the geometry of a contact relation is *not suitable as part of the twin definition*. Contact relations, however, play an important role for the morphological classification of twins (*cf.* Section 3.3.3.1). Frequently used alternative names for *twin boundaries* are *twin interfaces*, *contact planes*, *composition planes* or *domain boundaries*.

(5) Frequently, the term 'twin plane (*hkl*)' is used for the characterization of a *reflection twin*. This term is justified only if the twin mirror plane and the composition plane coincide. It is, however, ambiguous if the twin mirror plane and the twin interface have different orientations. In twins of hexagonal KLiSO$_4$, for example, the prominent composition plane (0001) is normal to the twin mirror plane (10$\bar{1}$0) (*cf.* Klapper *et al.*, 1987). The short term 'twin plane' should be avoided in such cases and substituted by *twin mirror plane* or *twin reflection plane*. The frequently used term 'twinning on (*hkl*)' [German: '*Zwillinge nach* (*hkl*)'] refers to (*hkl*) as a twin mirror plane and not as a contact plane.

(6) There exist twins in which the twin operations can be regarded as *fivefold* or *tenfold* rotations (Ellner & Burkhardt, 1993; Ellner, 1995). These twins are due to pseudo-pentagonal or pseudo-decagonal metrical features of the lattice [$\gamma = \arctan(c/a) \approx 72°$]. They can be treated in the same way as the three-, four- and sixfold rotation twins mentioned above. This includes the alternative ('exact') description of the twinning by a cyclic sequence of symmetrically equivalent twin reflection planes or twofold twin axes (*cf.* aragonite, Fig. 3.3.2.4). For this reason, we recommend that these intergrowths are accepted as (pseudo) *n*-fold rotation twins, even though the value of *n* is noncrystallographic.

(7) The classical treatment of twins considers only rotations, reflections and inversions as twin operations. In domain structures, relations between domain states exist that involve only *translations* (*cf.* Section 3.4.3), specifically those that are suppressed during a phase transition. Since every domain structure can be considered as a transformation twin, it seems legitimate to accept these translations as twin operations and speak of *translation twins* (T-twins according to Wadhawan, 1997, 2000). The translation vector of this twin operation is also known as the *fault vector* of the *translation boundary* (often called the *antiphase boundary*) between two *translation domains* [*cf.* Section 3.3.1(v)]. It must be realized, however, that the acceptance of translation domains as twins would classify all stacking faults in metals, in diamond and in semiconductors as twin boundaries.

(8) The structural consideration of twin boundaries cannot be performed by employing only point-group twin elements as is sufficient for the description of the orientation relation. In structural discussions, in addition, a translational displacement of the two structures with respect to each other by a shift vector, which is called here the *twin displacement vector* **t**, has to be taken into account. This displacement vector leads to a minimization of the twin-boundary energy. The components of this vector can have values between 0 and 1 of the basis vectors. In many cases, especially of transformation twins, glide planes or screw axes can occur as twin elements, whereby the glide or screw components may be relaxed, *i.e.* may deviate from their ideal values. The twin displacement vectors, as introduced here, include these glide or screw components and their relaxations. The role of the twin displacement vectors in the structure of the twin boundary is discussed in Section 3.3.10.4.

(9) In some cases the term 'twin' is used for systematic *oriented intergrowths* of crystals which are not twins as defined in this chapter. The following cases should be mentioned:

(i) *Allotwins* (Nespolo, Ferraris *et al.*, 1999): oriented crystal associations of different polytypes of the same compound. Different polytypes have the same chemistry and similar but nevertheless different structures. Well known examples are the micas, where twins and allotwins occur together (Nespolo *et al.*, 2000).

(ii) The oriented associations of two *polymorphs* (modifications) of the same compound across a phase boundary also do not deserve the name twin because of the different structures of their components. Note that this case is more general than the 'allotwins' of polytypes mentioned above. Interesting examples are the oriented intergrowths of the TiO$_2$ polymorphs rutile, anatase
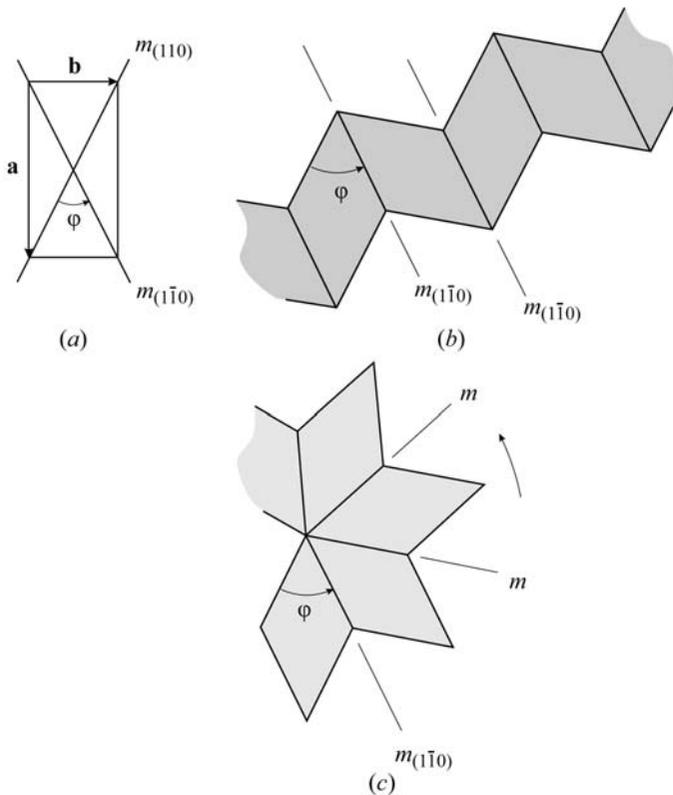
Fig. 3.3.3.1. Schematic illustration of simple (polysynthetic) and multiple (cyclic) twins. (a) Equivalent twin mirror planes (110) and (1$\bar{1}$0) of an orthorhombic crystal. (b) Simple (polysynthetic) twin with two orientation states due to parallel repetition of the same twin mirror plane (1$\bar{1}$0); the twin components are represented by {110} rhombs. (c) Multiple (cyclic) twin with several (more than two) orientation states due to cyclic repetition of equivalent twin mirror planes of type {110}.

and brookite. In this respect, the high-resolution transmission electron microscopy (HRTEM) studies of hydrothermally coarsened TiO$_2$ nanoparticles by Penn & Banfield (1998), showing the structures of anatase {121} reflection twin boundaries and of {112} anatase–(100) brookite interfaces on an atomic scale, are noteworthy.

(iii) *Plesiotwins* (Nespolo, Kogure & Ferraris, 1999): oriented crystal associations based on a large coincidence-site lattice (CSL). The composition plane has a low degree of restoration of lattice nodes and the relative rotations between individuals are noncrystallographic. In the phlogopite from Mutsure-jima, Japan, both ordinary twins and plesiotwins are reported (Sunagawa & Tomura, 1976).

3.3.3. Morphological classification, simple and multiple twinning

Before discussing the symmetry features of twinning in detail, it is useful to introduce the terms 'simple' and 'multiple' twins, which are sometimes grouped under the heading 'repetitive or repeated twins'. This is followed by some morphological aspects of twinning.

Simple twins are aggregates that consist of domains of only two orientation states, irrespective of the number, size and shape of the individual domains, Fig. 3.3.3.1(b). Thus, only one orientation relation (one twin law) exists. Contact twins and polysynthetic twins (see below) are simple twins.

Multiple twins are aggregates that contain domains of three or more orientation states, *i.e.* at least two twin laws are involved. Two cases have to be distinguished:

(i) The twin elements are symmetrically *equivalent* with respect to the *eigensymmetry* group $\mathcal{H}$ of the crystal (*cf.* Section 3.3.4.1). A typical example is provided by the equivalent (110) and (1$\bar{1}$0)

twin mirror planes of an orthorhombic crystal (*e.g.* aragonite), which frequently lead to *cyclic twins* (*cf.* Figs. 3.3.3.1a and c).

(ii) The twin elements are *not equivalent* with respect to the *eigensymmetry* of the crystal, *i.e.* several independent twin laws occur simultaneously in the twinned crystal. A typical example is provided by a Brazil twin of quartz, with each Brazil domain containing Dauphiné twins. This results in four domain states and three twin laws; *cf.* Example 3.3.6.3.

The distinction of simple and multiple twins is important for the following morphological classification. Further examples are given in Section 3.3.6.

3.3.3.1. Morphological classification

The morphology of twinned crystals, even for the same species and the same orientation relation, can be quite variable. For a given orientation relation the morphology depends on the geometry of the twin boundary as well as on the number of twin partners. A typical morphological feature of growth-twinned crystals is the occurrence of re-entrant angles. These angles are responsible for an increased growth velocity parallel to the twin boundary. This is the reason why twinned crystals often grow as platelets parallel to the composition plane (*cf.* Section 3.3.7.1). Detailed studies of the morphology of twins *versus* untwinned crystals were carried out as early as 1911 by Becke (1911). As a general observation, twinned crystals grow larger than untwinned crystals in the same batch.

The following classification of twins is in use:

(i) *Contact twins*. Two twin partners are in contact across a single composition plane $\pm(hkl)$, the Miller indices h, k, l of which have the same values for both partners ('common' plane). The contact plane usually has low indices. For reflection twins, the composition plane is frequently parallel to the twin mirror plane [see, however, Note (4) in Section 3.3.2.4]. Examples are shown in Fig. 3.3.6.1 for gypsum, in Fig. 3.3.6.5 for calcite and in Fig. 3.3.6.6(a) for a spinel (111) twin. In most cases, contact twins are growth twins.

(ii) *Polysynthetic (lamellar) twins* are formed by repetition of contact twins and consist of a linear sequence of domains with two alternating orientation states. The contact planes are parallel (lamellar twinning). This is typical for reflection twins if the twin mirror plane and the composition plane coincide. An illustrative example is the albite growth twin shown in Fig. 3.3.6.11. Polysynthetic twins may occur in growth, transformation and deformation twinning.

(iii) *Penetration twins*. The name 'penetration twin' results from the apparent penetration of two or more (idiomorphic) single crystals. The most prominent examples are twins of the spinel law in cubic crystals (*e.g.* spinels, fluorite, diamond). The spinel law is a reflection across (111) or a twofold rotation around [111]. Ideally these twins appear as two interpenetrating cubes with a common threefold axis, each cube representing one domain state (Fig. 3.3.6.6b). In reality, these twins usually consist of 12 pyramid-shaped domains, six of each domain state, all originating from a common point in the centre of the twinned crystal (as shown in Figs. 3.3.6.4 and 3.3.6.6). Another famous example is the Carlsbad twin of orthoclase feldspar with [001] as a twofold twin axis (Fig. 3.3.7.1). Penetration twins are always growth twins.

(iv) *Cyclic twins and sector twins*. In contrast to the linear sequence of domains in polysynthetic twins, *cyclic twins* form a circular arrangement of domains of suitable shape. They are always multiple twins (three or more orientations states) which are (formally) generated by successive application of equivalent twin laws. The twin aggregate may form a full circle or a fraction of a circle (see Figs. 3.3.3.1c, 3.3.6.7 and 3.3.6.10). Impressive examples are the 'sixlings' and 'eightlings' of rutile (Fig. 3.3.6.9, *cf.* Example 3.3.6.9).