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3.3. Twinning of crystals

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In this chapter, the basic concepts and definitions of twinning, as well as the morphological, genetic and lattice classifications of twins, are presented. Furthermore, twin boundaries are discussed extensively. The effect of twinning in reciprocal space, *i.e.* on diffraction and crystal-structure determinations, is outside the scope of the present edition. In the literature, the concept of twinning is very often used in a non-precise or ambiguous way. In order to clarify the terminology, this chapter begins with a section on the various kinds of crystal aggregates and intergrowths; in this context twinning appears as a special intergrowth with well defined crystallographic orientation relations.

3.3.1. Crystal aggregates and intergrowths

Minerals in nature and synthetic solid materials display different kinds of *aggregations*, in mineralogy often called *intergrowths*. In this chapter, we consider only aggregates of crystal grains of the same species, *i.e.* of the same (or nearly the same) chemical composition and crystal structure (homophase aggregates). Intergrowths of grains of different species (heterophase aggregates), *e.g.* heterophase bicrystals, epitaxy (two-dimensional oriented intergrowth on a surface), topotaxy (three-dimensional oriented precipitation or exsolution) or the paragenesis of different minerals in a rock or in a technical product are not treated in this chapter.

(i) *Arbitrary intergrowth*: Aggregation of two or more crystal grains with arbitrary orientation, *i.e.* without any systematic regularity. Examples are irregular aggregates of quartz crystals (*Bergkristall*) in a geode and intergrown single crystals precipitated from a solution. To this category also belong untextured polycrystalline materials and ceramics, as well as sandstone and quartzite.

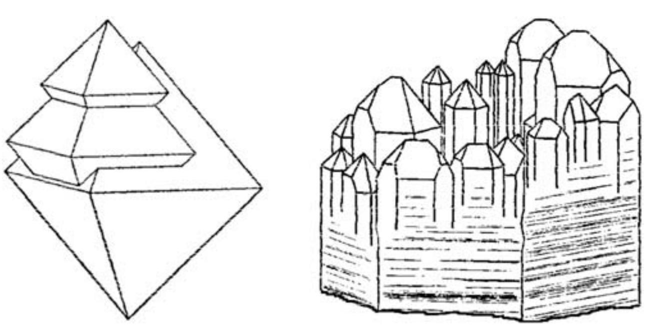
(ii) *Parallel intergrowth*: Combination of two or more crystals with parallel (or nearly parallel) orientation of all edges and faces. Examples are dendritic intergrowths as well as parallel intergrowths of spinel octahedra (Fig. 3.3.1.1*a*) and of quartz prisms (Fig. 3.3.1.1*b*). Parallel intergrowths frequently exhibit re-entrant angles and are, therefore, easily misinterpreted as twins.

In this context the term *mosaic crystal* must be mentioned. It was introduced in the early years of X-ray diffraction in order to characterize the perfection of a crystal. A mosaic crystal consists of small blocks (size typically in the micron range) with orientations deviating only slightly from the average orientation of the crystal; the term 'lineage structure' is also used for very small scale parallel intergrowths (Buerger, 1934, 1960*a*, pp. 69–73).

(iii) *Bicrystals*: This term is mainly used in metallurgy. It refers to the (usually synthetic) intergrowth of two single crystals with a well defined orientation relation. A bicrystal contains a *grain boundary*, which in general is also well defined. Usually, homophase bicrystals are synthesized in order to study the structure and properties of grain boundaries. An important tool for the theoretical treatment of bicrystals and their interfaces is the *coincidence-site lattice* (CSL). A brief survey of bicrystals is given in Section 3.2.2; a comparison with twins and domain structures is provided by Hahn *et al*. (1999).

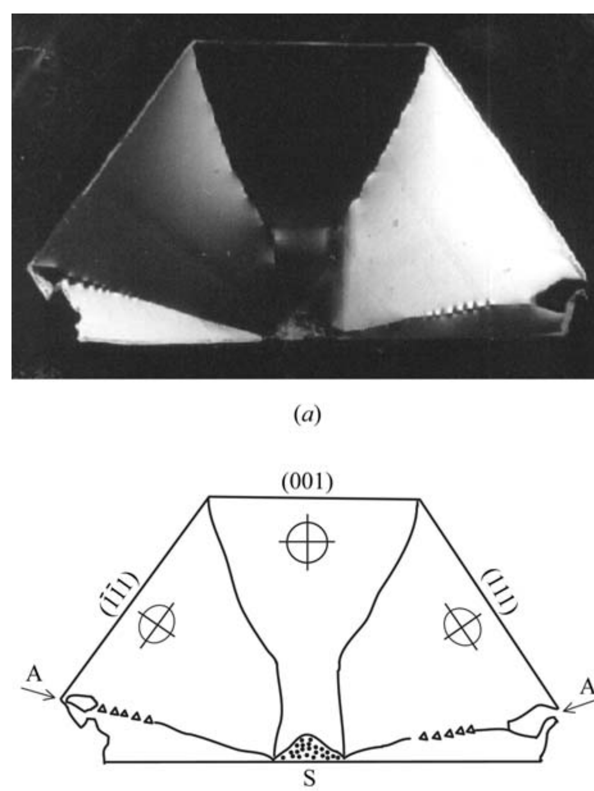
(iv) *Growth sectors*: Crystals grown with planar faces (habit faces), *e.g.* from vapour, supercooled melt or solution, consist of regions crystallized on different growth faces (Fig. 3.3.1.2). These growth sectors usually have the shapes of pyramids with their apices pointing toward the nucleus or the seed crystal. They are separated by *growth-sector boundaries*, which represent inner surfaces swept by the crystal edges during growth. In many cases, these boundaries are imperfections of the crystal.

Frequently, the various growth sectors of one crystal exhibit slightly different chemical and physical properties. Of particular



(*a*) (*b*)

Fig. 3.3.1.1. Parallel intergrowth (*a*) of spinel octahedra and (*b*) of hexagonal quartz prisms. Part (*a*) after Phillips (1971, p. 172), part (*b*) after Tschermak & Becke (1915, p. 94).



(*a*)

(*b*)

Fig. 3.3.1.2. (*a*) Optical anomaly of a cubic mixed (K,NH_4)-alum crystal grown from aqueous solution, as revealed by polarized light between crossed polarizers: (110) plate, 1 mm thick, horizontal dimension about 4 cm. (*b*) Sketch of growth sectors and their boundaries of the crystal plate shown in (*a*). The {111} growth sectors are optically negative and approximately uniaxial with their optical axes parallel to their growth directions ⟨111⟩ [birefringence Δn up to 5×10^{-5}; Shtukenberg *et al.* (2001)]. The (001) growth sector is nearly isotropic ($\Delta n < 10^{-6}$). Along the boundaries A between {111} sectors a few small {110} growth sectors (resulting from small {110} facets) have formed during growth. S: seed crystal.

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 ⟨100⟩ 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.* $[uvw]_{\rm I}$ is parallel to $\pm[uvw]_{\rm II}$;

(ii) at least *two* lattice planes (crystal faces) $(hkl)_{\rm I}$ and $\pm(hkl)_{\rm II}$, 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

references