

### 3.3. Twinning of crystals

BY TH. HAHN AND H. KLAPPER

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

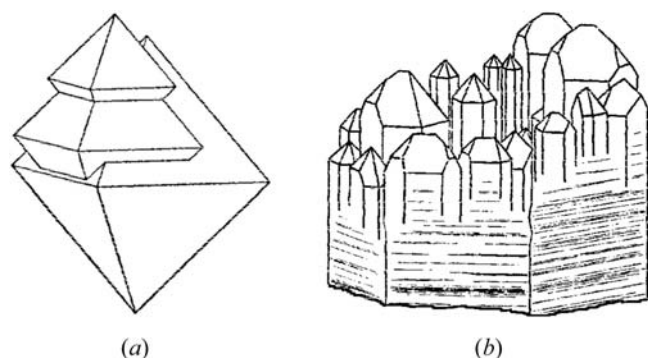


Fig. 3.3.1.1. Parallel intergrowth (a) of spinel octahedra and (b) of hexagonal quartz prisms. Part (a) after Phillips (1971, p. 172), part (b) after Tschermak & Becke (1915, p. 94).

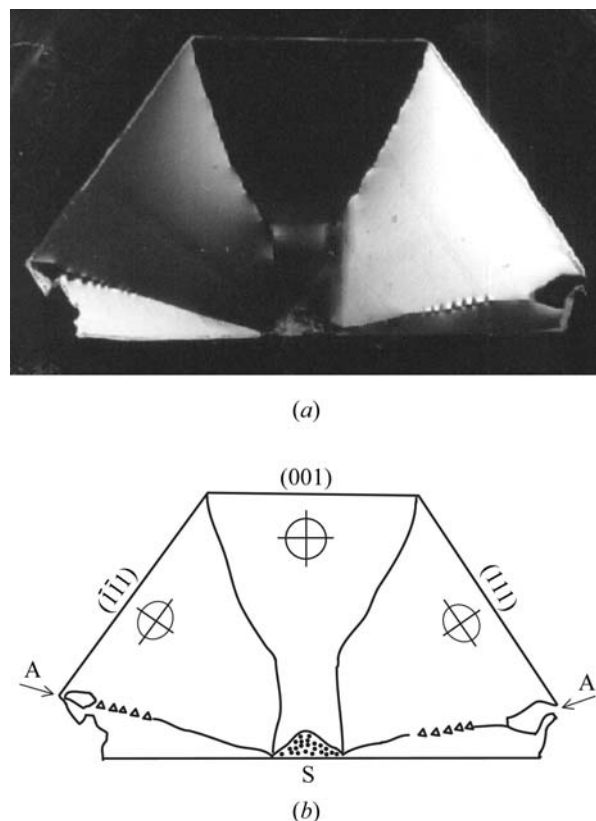


Fig. 3.3.1.2. (a) Optical anomaly of a cubic mixed (K,NH<sub>4</sub>)-alum crystal grown from aqueous solution, as revealed by polarized light between crossed polarizers: (110) plate, 1 mm thick, horizontal dimension about 4 cm. (b) Sketch of growth sectors and their boundaries of the crystal plate shown in (a). The {111} growth sectors are optically negative and approximately uniaxial with their optical axes parallel to their growth directions (111) [birefringence  $\Delta n$  up to  $5 \times 10^{-5}$ ; 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.