International Tables for Crystallography (2013). Vol. D, Section 3.4.4.1, pp. 528–529.

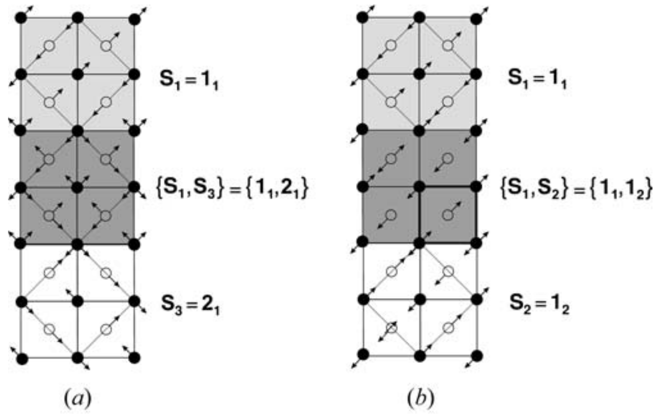

Fig. 3.4.3.10. Domain pairs in calomel. Single-domain states in the parent clamping approximation are those from Fig. 3.4.2.5. The first domain state of a domain pair is shown shaded in grey ('black'), the second domain state is colourless ('white'), and the domain pair of two interpenetrating domain states is shown shaded in dark grey. (*a*) Ferroelastic domain pair (S_1, S_3) in the parent clamping approximation. This is a partially transposable domain pair. (*b*) Translational domain pair (S_1, S_2). This is a completely transposable domain pair.

Example 3.4.3.8. Ferroelastic crystal of langbeinite. Langbeinite $K_2Mg_2(SO_4)_3$ undergoes a phase transition with symmetry descent $23 \supset 222$ that appears in Table 3.4.3.7. The ferroelastic phase has three ferroelastic domain states. Dudnik & Shuvalov (1989) found, in accord with their theoretical predictions, nearly linear 'almost coherent' domain walls accompanied by elastic stresses in crystals thinner than 0.5 mm. In thicker crystals, elastic stresses became so large that crystals were cracking and no domain walls were observed.

Similar effects were reported by the same authors for the partial ferroelastic phase of $CH_3NH_3Al(SO_4)_2{\cdot}12H_2O$ (MASD) with symmetry descent $\bar{3}m \supset mmm$, where ferroelastic domain walls were detected only in thin samples.

3.4.3.7. *Domain pairs in the microscopic description*

In the *microscopic description*, two microscopic domain states S_i and S_k with space-group symmetries $\mathcal{F}_i$ and $\mathcal{F}_k$, respectively, can form an ordered domain pair (S_i, S_k) and an unordered domain pair $\{S_i, S_k\}$ in a similar way to in the continuum description, but one additional aspect has to be considered. The definition of the symmetry group $\mathcal{F}_{ik}$ of an ordered domain pair (S_i, S_k),

$$\mathcal{F}_{ik} = \mathcal{F}_i \cap \mathcal{F}_k, \qquad (3.4.3.72)$$

is meaningful only if the group $\mathcal{F}_{ik}$ is a space group with a three-dimensional translational subgroup (three-dimensional *twin lattice* in the classical description of twinning, see Section 3.3.8)

$$\mathcal{T}_{ik} = \mathcal{T}_i \cap \mathcal{T}_k, \qquad (3.4.3.73)$$

where $\mathcal{T}_i$ and $\mathcal{T}_k$ are translation subgroups of $\mathcal{F}_i$ and $\mathcal{F}_k$, respectively. This condition is fulfilled if both domain states S_i and S_k have the same spontaneous strains, *i.e.* in non-ferroelastic domain pairs, but in ferroelastic domain pairs one has to suppress spontaneous deformations by applying the parent clamping approximation [see Section 3.4.2.2, equation (3.4.2.49)].

Example 3.4.3.9. Domain pairs in calomel. Calomel undergoes a non-equitranslational phase transition from a tetragonal parent phase to an orthorhombic ferroelastic phase (see Example 3.4.2.7 in Section 3.4.2.5). Four basic microscopic single-domain states are displayed in Fig. 3.4.2.5. From these states, one can form 12 non-trivial ordered single-domain pairs that can be partitioned (by means of double coset decomposition) into two orbits of domain pairs.

Representative domain pairs of these orbits are depicted in Fig. 3.4.3.10, where the first microscopic domain state S_i participating in a domain pair is displayed in the upper cell (light grey) and the second domain state S_j, $j = 2, 3$, in the lower white cell. The overlapping structure in the middle (dark grey) is a geometrical representation of the domain pair $\{S_1, S_j\}$.

The domain pair $\{S_1, S_3\}$, depicted in Fig. 3.4.3.10(*a*), is a ferroelastic domain pair in the parent clamping approximation. Then two overlapping structures of the domain pair have a common three-dimensional lattice with a common unit cell (the dotted square), which is the same as the unit cells of domain states S_1 and S_3.

Domain pair $\{S_1, S_2\}$, shown in Fig. 3.4.3.10(*b*), is a translational (antiphase) domain pair in which domain states S_1 and S_2 differ only in location but not in orientation. The unit cell (heavily outlined small square) of the domain pair $\{S_1, S_2\}$ is identical with the unit cell of the tetragonal parent phase (*cf.* Fig. 3.4.2.5).

The two arrows attached to the circles in the domain pairs represent exaggerated displacements within the wall.

Domain pairs represent an intermediate step in analyzing microscopic structures of domain walls, as we shall see in Section 3.4.4.

3.4.4. Domain twins and domain walls

3.4.4.1. *Formal description of simple domain twins and planar domain walls of zero thickness*

In this section, we examine crystallographic properties of planar compatible domain walls and simple domain twins. The symmetry of these objects is described by layer groups. Since this concept is not yet common in crystallography, we briefly explain its meaning in Section 3.4.4.2. The exposition is performed in the continuum description, but most of the results apply with slight generalizations to the microscopic treatment that is illustrated with an example in Section 3.4.4.7.

We shall consider a *simple domain twin* $\mathbf{T}_{12}$ that consists of two domains $\mathbf{D}_1$ and $\mathbf{D}_2$ which meet along a planar domain wall $\mathbf{W}_{12}$ of zero thickness. Let us denote by p a *plane of the domain wall*, in brief *wall plane* of $\mathbf{W}_{12}$. This plane is specified by Miller indices (hkl), or by a normal $\mathbf{n}$ to the plane which also defines the sidedness (plus and minus side) of the plane p. By *orientation of the plane p* we shall understand a specification which can, but may not, include the sidedness of p. If both the orientation and the sidedness are given, then the plane p divides the space into two half-spaces. Using the bra–ket symbols, mentioned in Section 3.4.3.6, we shall denote by $(\,|$ the half-space on the negative side of p and by $|\,)$ the half-space on the positive side of p.

A *simple twin* consists of two (theoretically semi-infinite) domains $\mathbf{D}_1$ and $\mathbf{D}_2$ with domain states $\mathbf{S}_1$ and $\mathbf{S}_2$, respectively, that join along a planar domain wall the orientation of which is specified by the wall plane p with normal $\mathbf{n}$. A symbol $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_2)$ specifies the domain twin unequivocally: domain $(\mathbf{S}_1|$, with domain region $(\,|$ filled with domain state $\mathbf{S}_1$, is on the negative side of p and domain $|\,\mathbf{S}_2)$ is on the positive side of p (see Fig. 3.4.4.1*a*).

If we were to choose the normal of opposite direction, *i.e.* $-\mathbf{n}$, the same twin would have the symbol $(\mathbf{S}_2|-\mathbf{n}|\mathbf{S}_1)$ (see Fig. 3.4.4.1*a*). Since these two symbols signify the same twin, we have the identity

$$(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_2) \equiv (\mathbf{S}_2|-\mathbf{n}|\mathbf{S}_1). \qquad (3.4.4.1)$$

Thus, if we invert the normal $\mathbf{n}$ and simultaneously exchange domain states $\mathbf{S}_1$ and $\mathbf{S}_2$ in the twin symbol, we obtain an identical twin (see Fig. 3.4.4.1*a*). This identity expresses the fact that the

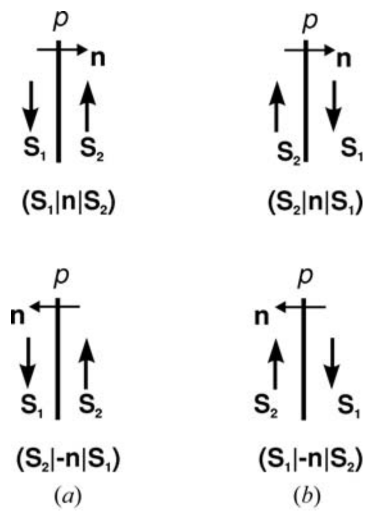

Fig. 3.4.4.1. Symbols of a simple twin. (*a*) Two different symbols with antiparallel normal **n**. (*b*) Symbols of the reversed twin.

specification of the twin by the symbol introduced above does not depend on the chosen direction of the wall normal **n**.

The full symbol of the twin can be replaced by a shorter symbol $\mathbf{T}_{12}(\mathbf{n})$ if we accept a simple convention that the first lower index signifies the domain state that occupies the half space (| on the negative side of **n**. Then the identity (3.4.4.1) in short symbols is

$$\mathbf{T}_{12}(\mathbf{n}) \equiv \mathbf{T}_{21}(-\mathbf{n}). \quad (3.4.4.2)$$

If the orientation and sidedness of the plane p of a wall is known from the context or if it is not relevant, the specification of **n** in the symbol of the domain twin and domain wall can be omitted.

A twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_2)$, or $\mathbf{T}_{12}(\mathbf{n})$, can be formed by sectioning the ordered domain pair $(\mathbf{S}_1, \mathbf{S}_2)$ by a plane p with normal **n** and removing the domain state $\mathbf{S}_2$ on the negative side and domain state $\mathbf{S}_2$ on the positive side of the normal **n**. This is the same procedure that is used in bicrystallography when an ideal bicrystal is derived from a dichromatic complex (see Section 3.2.2).

A twin with reversed order of domain states is called a *reversed twin*. The symbol of the twin reversed to the initial twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_2)$ is

$$(\mathbf{S}_2|\mathbf{n}|\mathbf{S}_1) \equiv (\mathbf{S}_1| - \mathbf{n}|\mathbf{S}_2) \quad (3.4.4.3)$$

or

$$\mathbf{T}_{21}(\mathbf{n}) \equiv \mathbf{T}_{12}(-\mathbf{n}). \quad (3.4.4.4)$$

A reversed twin $(\mathbf{S}_2|\mathbf{n}|\mathbf{S}_1) \equiv (\mathbf{S}_1|-\mathbf{n}|\mathbf{S}_2)$ is depicted in Fig. 3.4.4.1(*b*).

A *planar domain wall* is the interface between the domains $\mathbf{D}_1$ and $\mathbf{D}_2$ of the associated simple twin. Even a domain wall of zero thickness is specified not only by its orientation in space but also by the domain states that adhere to the minus and plus sides of the wall plane p. The symbol for the wall is, therefore, analogous to that of the twin, only in the explicit symbol the brackets ( ) are replaced by square brackets [ ] and **T** in the short symbol is replaced by **W**:

$$[\mathbf{S}_1|\mathbf{n}|\mathbf{S}_2] \equiv [\mathbf{S}_2| - \mathbf{n}|\mathbf{S}_1] \quad (3.4.4.5)$$

or by a shorter equivalent symbol

$$\mathbf{W}_{12}(\mathbf{n}) \equiv \mathbf{W}_{21}(-\mathbf{n}). \quad (3.4.4.6)$$

3.4.4.2. *Layer groups*

An adequate concept for characterizing symmetry properties of simple domain twins and planar domain walls is that of layer groups. A layer group describes the symmetry of objects that exist in a three-dimensional space and have two-dimensional translation symmetry. Typical examples are two-dimensional planes in three-dimensional space [two-sided planes and sectional layer groups (Holser, 1958*a*,*b*), domain walls and interfaces of zero thickness], layers of finite thickness (*e.g.* domain walls and interfaces of finite thickness) and two semi-infinite crystals joined along a planar and coherent (compatible) interface [*e.g.* simple domain twins with a compatible (coherent) domain wall, bicrystals].

A *crystallographic layer group* comprises symmetry operations (isometries) that leave invariant a chosen crystallographic plane p in a crystalline object. There are two types of such operations:

(i) *side-preserving operations* keep invariant the normal **n** of the plane p, *i.e.* map each side of the plane p onto the same side. This type includes translations (discrete or continuous) in the plane p, rotations of $360°/n$, $n = 2, 3, 4, 6$, around axes perpendicular to the plane p, reflections through planes perpendicular to p and glide reflections through planes perpendicular to p with glide vectors parallel to p. The corresponding symmetry elements are not related to the location of the plane p in space, *i.e.* they are the same for all planes parallel to p.

(ii) *side-reversing operations* invert the normal **n** of the plane *i.e.* exchange sides of the plane. Operations of this type are: an inversion through a point in the plane p, rotations of $360°/n$, $n = 3, 4, 6$ around axes perpendicular to the plane followed by inversion through this point, 180° rotation and 180° screw rotation around an axis in the plane p, reflection and glide reflections through the plane p, and combinations of these operations with translations in the plane p. All corresponding symmetry elements are located in the plane p.

A layer group $\mathcal{L}$ consists of two parts:

$$\mathcal{L} = \widehat{\mathcal{L}} \cup \underline{s}\widehat{\mathcal{L}}, \quad (3.4.4.7)$$

where $\widehat{\mathcal{L}}$ is a subgroup of $\mathcal{L}$ that comprises all side-preserving operations of $\mathcal{L}$; this group is isomorphic to a plane group and is called a *trivial layer group* or a *face group*. An underlined character $\underline{s}$ denotes a side-reversing operation and the left coset $\underline{s}\widehat{\mathcal{L}}$ contains all side-reversing operations of $\mathcal{L}$. Since $\widehat{\mathcal{L}}$ is a halving subgroup, the layer group $\mathcal{L}$ can be treated as a dichromatic (black-and-white) group in which side-preserving operations are colour-preserving operations and side-reversing operations are colour-exchanging operations.

There are 80 layer groups with discrete two-dimensional translation subgroups [for a detailed treatment see *IT* E (2010), or *e.g.* Vainshtein (1994), Shubnikov & Kopcik (1974), Holser (1958*a*)]. Equivalent names for these layer groups are *net groups* (Opechowski, 1986), *plane groups in three dimensions* (Grell *et al.*, 1989), *groups in a two-sided plane* (Holser, 1958*a*,*b*) and others.

To these layer groups there correspond 31 point groups that describe the symmetries of crystallographic objects with two-dimensional continuous translations. Holser (1958*b*) calls these groups *point groups in a two-sided plane*, Kopský (1993) coins the term *point-like layer groups*. We shall use the term 'layer groups' both for layer groups with discrete translations, used in a microscopic description, and for crystallographic 'point-like layer groups' with continuous translations in the continuum approach. The geometrical meaning of these groups is similar and most of the statements and formulae hold for both types of layer groups.

Crystallographic layer groups with a continuous translation group [point groups of two-sided plane (Holser, 1958*b*)] are listed in Table 3.4.4.1. The *international notation* corresponds to international symbols of layer groups with discrete translations; this notation is based on the Hermann–Mauguin (international)