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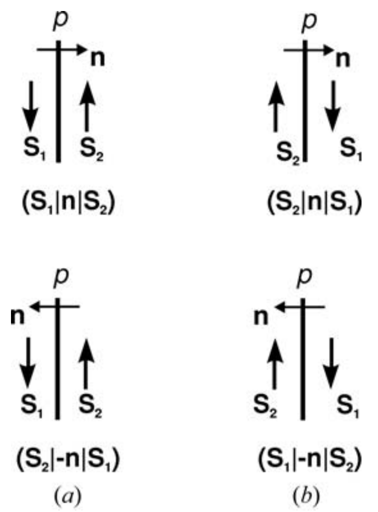

Fig. 3.4.4.1. Symbols of a simple twin. (*a*) Two different symbols with antiparallel normal **n**. (*b*) Symbols of the reversed twin.

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

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

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

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

or

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

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**:

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

or by a shorter equivalent symbol

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

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:

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

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)

Table 3.4.4.1. *Crystallographic layer groups with continuous translations*

International	Non-coordinate
1	1
$\bar{1}$	$\underline{\bar{1}}$
112	2
$11m$	$\underline{m}$
$112/m$	$2/\underline{m}$
211	$\underline{2}$
$m11$	$\underline{m}$
$2/m11$	$\underline{2}/m$
222	$\underline{22}2$
$mm2$	$mm2$
$m2m$	$m\underline{2m}$
mmm	$mm\underline{m}$
4	4
$\bar{4}$	$\underline{\bar{4}}$
$4/m$	$4/\underline{m}$
422	$4\underline{22}$
$4mm$	$4mm$
$\bar{4}2m$	$\underline{\bar{4}2}m$
$4/mmm$	$4/\underline{m}mm$
3	3
$\bar{3}$	$\underline{\bar{3}}$
32	$3\underline{2}$
$3m$	$3m$
$\bar{3}m$	$\underline{\bar{3}}m$
6	6
$\bar{6}$	$\underline{\bar{6}}$
$6/m$	$6/\underline{m}$
622	$6\underline{22}$
$6mm$	$6mm$
$\bar{6}m2$	$\underline{\bar{6}}m\underline{2}$
$6/mmm$	$6/\underline{m}mm$

symbols of three-dimensional space groups, where the c direction is the direction of missing translations and the character '1' represents a symmetry direction in the plane with no associated symmetry element (see *IT* E, 2010).

In the *non-coordinate notation* (Janovec, 1981), side-reversing operations are underlined. Thus *e.g.* $\underline{2}$ denotes a 180° rotation around a twofold axis in the plane p and $\underline{m}$ a reflection through this plane, whereas 2 is a side-preserving 180° rotation around an axis perpendicular to the plane and m is a side-preserving reflection through a plane perpendicular to the plane p. With exception of $\underline{\bar{1}}$ and $\underline{2}$, the symbol of an operation specifies the orientation of the plane p. This notation allows one to signify layer groups with different orientations in one reference coordinate system. Another non-coordinate notation has been introduced by Shubnikov & Kopcik (1974).

If a crystal with point-group symmetry G is bisected by a crystallographic plane p, then all operations of G that leave the plane p invariant form a *sectional layer group* = $\overline{\mathsf{G}(p)}$ *of the plane p in G*. Operations of the group $\overline{\mathsf{G}(p)}$ can be divided into two sets [see equation (3.4.4.7)]:

$$\overline{\mathsf{G}(p)} = \widehat{\mathsf{G}(p)} \,\cup\, \underline{g}\widehat{\mathsf{G}(p)}, \qquad (3.4.4.8)$$

where the trivial layer group $\widehat{\mathsf{G}(p)}$ expresses the symmetry of the crystal face with normal $\mathbf{n}$. These face symmetries are listed in *IT* A (2005), Part 10, for all crystallographic point groups G and all orientations of the plane expressed by Miller indices (hkl). The underlined operation $\underline{g}$ is a side-reversing operation that inverts the normal $\mathbf{n}$. The left coset $\underline{g}\widehat{\mathsf{G}(p)}$ contains all side-reversing operations of $\overline{\mathsf{G}(p)}$.

The number n_p of planes symmetry-equivalent (in G) with the plane p is equal to the index of $\overline{\mathsf{G}(p)}$ in G:

$$n_p = [G : \overline{\mathsf{G}(p)}] = |G| : |\overline{\mathsf{G}(p)}|. \qquad (3.4.4.9)$$

Example 3.4.4.1. As an example, we find the sectional layer group of the plane (010) in the group $G = 4_z/m_zm_xm_{xy}$ (see Fig. 3.4.2.2).

$$\begin{aligned} 4_z/m_zm_xm_{xy}(010) &= m_x2_ym_z \cup \underline{m}_y\{m_x2_ym_z\} \\ &= m_x2_ym_z \cup \{\underline{m}_y, \underline{2}_z, \underline{\bar{1}}, \underline{2}_x\} \\ &= m_x\underline{m}_ym_z. \end{aligned} \qquad (3.4.4.10)$$

In this example $n_p = |4_z/m_zm_xm_{xy}| : |m_x\underline{m}_ym_z| = 16 : 8 = 2$ and the plane crystallographically equivalent with the plane (010) is the plane (100) with sectional symmetry $\underline{m}_xm_ym_z$.

3.4.4.3. *Symmetry of simple twins and planar domain walls of zero thickness*

We shall examine the symmetry of a twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$ with a planar zero-thickness domain wall with orientation and location defined by a plane p (Janovec, 1981; Zikmund, 1984; Zieliński, 1990). The symmetry properties of a planar domain wall $\mathbf{W}_{1j}$ are the same as those of the corresponding simple domain twin. Further, we shall consider twins but all statements also apply to the corresponding domain walls.

Operations that express symmetry properties of the twin must leave the orientation and location of the plane p invariant. We shall perform our considerations in the continuum description and shall assume that the plane p passes through the origin of the coordinate system. Then point-group symmetry operations leave the origin invariant and do not change the position of p.

If we apply an operation $g \in G$ to the twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$, we get a crystallographically equivalent twin $(\mathbf{S}_i|\mathbf{n}_m|\mathbf{S}_k) \overset{G}{\sim} (\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$ with other domain states and another orientation of the domain wall,

$$g(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j) = (g\mathbf{S}_1|g\mathbf{n}|g\mathbf{S}_j) = (\mathbf{S}_i|\mathbf{n}_m|\mathbf{S}_k), \quad g \in G. \qquad (3.4.4.11)$$

It can be shown that the transformation of a domain pair by an operation $g \in G$ defined by this relation fulfils the conditions of an action of the group G on a set of all domain pairs formed from the orbit $G\mathbf{S}_1$ (see Section 3.2.3.3). We can, therefore, use all concepts (stabilizer, orbit, class of equivalence *etc.*) introduced for domain states and also for domain pairs.

Operations g that describe symmetry properties of the twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$ must not change the orientation of the wall plane p but can reverse the sides of p, and must either leave invariant both domain states $\mathbf{S}_1$ and $\mathbf{S}_j$ or exchange these two states. There are four types of such operations and their action is summarized in Table 3.4.4.2. It is instructive to follow this action in Fig. 3.4.4.2 using an example of the twin $(\mathbf{S}_1[010]\mathbf{S}_2)$ with domain states $\mathbf{S}_1$ and $\mathbf{S}_2$ from our illustrative example (see Fig. 3.4.2.2).

(1) An operation f_{1j} which leaves invariant the normal $\mathbf{n}$ and both domain states $\mathbf{S}_1$, $\mathbf{S}_j$ in the twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$; such an operation does not change the twin and is called the *trivial symmetry operation of the twin*. An example of such an operation of the twin $(\mathbf{S}_1[010]\mathbf{S}_2)$ in Fig. 3.4.4.2 is the reflection m_z.

(2) An operation $\underline{s}_{1j}$ which inverts the normal $\mathbf{n}$ but leaves invariant both domain states $\mathbf{S}_1$ and $\mathbf{S}_j$. This *side-reversing* operation transforms the initial twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$ into $(\mathbf{S}_1|-\mathbf{n}|\mathbf{S}_j)$, which is, according to (3.4.4.1), identical with the inverse twin $(\mathbf{S}_j|\mathbf{n}|\mathbf{S}_1)$. As in the non-coordinate notation of layer groups (see Table 3.4.4.1) we shall underline the side-reversing operations. The reflection $\underline{m}_y$ in Fig. 3.4.4.2 is an example of a side-reversing operation.

(3) An operation $r^{\star}_{1j}$ which exchanges domain states $\mathbf{S}_1$ and $\mathbf{S}_j$ but does not change the normal $\mathbf{n}$. This *state-exchanging operation*, denoted by a star symbol, transforms the initial twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$ into a reversed twin $(\mathbf{S}_j|\mathbf{n}|\mathbf{S}_1)$. A state-exchanging operation in our example is the reflection $m^{\star}_x$.

references