International Tables for Crystallography (2013). Vol. D, Section 3.4.4.3, pp. 530–533.

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	$\underline{2}\underline{2}2$
$mm2$	$mm2$
$m2m$	$m\underline{2}\underline{m}$
mmm	$mm\underline{m}$
4	4
$\bar{4}$	$\underline{\bar{4}}$
$4/m$	$4/\underline{m}$
422	$4\underline{2}\underline{2}$
$4mm$	$4mm$
$\bar{4}2m$	$\underline{\bar{4}}\underline{2}m$
$4/mmm$	$4/\underline{m}mm$
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	$6\underline{2}\underline{2}$
$6mm$	$6mm$
$\bar{6}m2$	$\underline{\bar{6}}m\underline{2}$
$6/mmm$	$6/\underline{m}mm$

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 $G = 4_z/m_z m_x m_{xy}$ (see Fig. 3.4.2.2).

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

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

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 $m^{\star}_x$.

Table 3.4.4.2. *Action of four types of operations g on a twin* $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$

Operation g keeps the orientation of the plane p unchanged.

g	$g\mathbf{S}_1$	$g\mathbf{S}_j$	$g\mathbf{n}$	$g(\mathbf{S}_1|$	$g|\mathbf{S}_j)$	$g(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j) = (g\mathbf{S}_1|g\mathbf{n}|g\mathbf{S}_j)$	Resulting twin
f_{1j}	$\mathbf{S}_1$	$\mathbf{S}_j$	$\mathbf{n}$	$(\mathbf{S}_1|$	$|\mathbf{S}_j)$	$(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$	Initial twin
$\underline{s}_{1j}$	$\mathbf{S}_1$	$\mathbf{S}_j$	$-\mathbf{n}$	$|\mathbf{S}_1)$	$(\mathbf{S}_j|$	$(\mathbf{S}_1|-\mathbf{n}|\mathbf{S}_j) \equiv (\mathbf{S}_j|\mathbf{n}|\mathbf{S}_1)$	Reversed twin
$r^\star_{1j}$	$\mathbf{S}_j$	$\mathbf{S}_1$	$\mathbf{n}$	$(\mathbf{S}_j|$	$|\mathbf{S}_1)$	$(\mathbf{S}_j|\mathbf{n}|\mathbf{S}_1)$	Reversed twin
$\underline{t}^\star_{1j}$	$\mathbf{S}_j$	$\mathbf{S}_1$	$-\mathbf{n}$	$|\mathbf{S}_j)$	$(\mathbf{S}_1|$	$(\mathbf{S}_j|-\mathbf{n}|\mathbf{S}_1) \equiv (\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$	Initial twin

(4) An operation $\underline{t}^\star_{1j}$ which inverts $\mathbf{n}$ and simultaneously exchanges $\mathbf{S}_1$ and $\mathbf{S}_j$. This operation, called the *non-trivial symmetry operation of a twin*, transforms the initial twin into $(\mathbf{S}_j|-\mathbf{n}|\mathbf{S}_1)$, which is, according to (3.4.4.1), identical with the initial twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$. An operation of this type can be expressed as a product of a side-exchanging operation (underlined) and a state-exchanging operation (with a star), and will, therefore, be underlined and marked by a star. In Fig. 3.4.4.2, a non-trivial symmetry operation is for example the 180° rotation $\underline{2}^\star_z$.

We note that the star and the underlining do not represent any operation; they are just suitable auxiliary labels that can be omitted without changing the result of the operation.

To find all trivial symmetry operations of the twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$, we recall that all symmetry operations that leave both $\mathbf{S}_1$ and $\mathbf{S}_j$ invariant constitute the symmetry group F_{1j} of the ordered domain pair $(\mathbf{S}_1, \mathbf{S}_j)$, $F_{1j} = F_1 \cap F_j$, where F_1 and F_j are the symmetry groups of $\mathbf{S}_1$ and $\mathbf{S}_j$, respectively. The sectional layer group of the plane p in group F_{1j} is (if we omit p)

$$\overline{\mathsf{F}}_{1j} = \widehat{\mathsf{F}}_{1j} \cup \underline{s}_{1j}\widehat{\mathsf{F}}_{1j}. \qquad (3.4.4.12)$$

The trivial (side-preserving) subgroup $\widehat{\mathsf{F}}_{1j}$ assembles all trivial symmetry operations of the twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$. The left coset $\underline{s}_{1j}\widehat{\mathsf{F}}_{1j}$, where $\underline{s}_{1j}$ is a side-reversing operation, contains all side-reversing operations of this twin. In our example $\widehat{F}_{12} = \{1, m_z\}$ and $\underline{s}_{1j}\widehat{\mathsf{F}}_{1j} = \underline{m}_y\{1, m_z\} = \{\underline{m}_y, \underline{2}_x\}$ (see Fig. 3.4.4.2).

Similarly, the left coset $r^\star_{1j}\widehat{\mathsf{F}}_{1j}$ contains all state-exchanging operations, and $\underline{t}^\star_{1j}\widehat{\mathsf{F}}_{1j}$ all non-trivial symmetry operations of the twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$. In the illustrative example, $r^\star_{1j}\widehat{\mathsf{F}}_{1j} = m^\star_x\{1, m_z\} = \{m^\star_x, 2^\star_y\}$ and $\underline{t}^\star_{1j}\widehat{\mathsf{F}}_{1j} = \underline{2}^\star_z\{1, m_z\} = \{\underline{2}^\star_z, \underline{\bar{1}}^\star\}$.

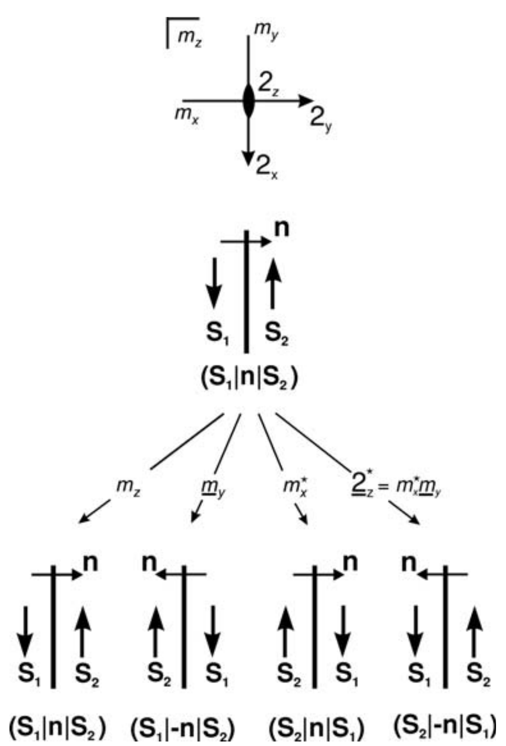

Fig. 3.4.4.2. A simple twin under the action of four types of operation that do not change the orientation of the wall plane p. Compare with Table 3.4.4.2.

The trivial group $\widehat{F}_{1j}$ and its three cosets constitute the sectional layer group $\overline{J}_{1j}$ of the plane p in the symmetry group $J_{1j} = F_{1j} \cup g^\star_{1j}F_{1j}$ of the unordered domain pair $\{\mathbf{S}_1, \mathbf{S}_j\}$,

$$\overline{\mathsf{J}}_{1j} = \widehat{\mathsf{J}}_{1j} \cup \underline{s}_{1j}\widehat{\mathsf{J}}_{1j} = \widehat{\mathsf{F}}_{1j} \cup r^\star_{1j}\widehat{\mathsf{F}}_{1j} \cup \underline{s}_{1j}\widehat{\mathsf{F}}_{1j} \cup \underline{t}^\star_{1j}\widehat{\mathsf{F}}_{1j}, \qquad (3.4.4.13)$$

where $r^\star_{1j}$ is an operation of the left coset $g^\star_{1j}F_{1j}$ that leaves the normal $\mathbf{n}$ invariant and $\underline{t}^*_{1j} = \underline{s}_{1j}r^\star_{1j}$.

Group $\overline{\mathsf{J}}_{1j}$ can be interpreted as a symmetry group of a *twin pair* $(\mathbf{S}_1, \mathbf{S}_j|\mathbf{n}|\mathbf{S}_j, \mathbf{S}_1)$ consisting of a domain twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$ and a superposed reversed twin $(\mathbf{S}_j|\mathbf{n}|\mathbf{S}_1)$ with a common wall plane p. This construct is analogous to a domain pair (dichromatic complex in bicrystallography) in which two homogeneous domain states $\mathbf{S}_1$ and $\mathbf{S}_j$ are superposed (see Section 3.4.3.1). In the same way as the group J_{1j} of domain pair $\{\mathbf{S}_1, \mathbf{S}_j\}$ is divided into two cosets with different results of the action on this domain pair, the symmetry group $\overline{\mathsf{J}}_{1j}$ of the twin pair can be decomposed into four cosets (3.4.4.13), each of which acts on a domain twin $(\mathbf{S}_j|\mathbf{n}|\mathbf{S}_1)$ in a different way, as specified in Table 3.4.4.2.

We can associate with operations from each coset in (3.4.4.13) a label. If we denote operations from $\widehat{\mathsf{F}}_{1j}$ without a label by e, underlining by a and star by b, then the multiplication of labels is expressed by the relations

$$a^2 = b^2 = e, \quad ab = ba. \qquad (3.4.4.14)$$

The four different labels e, a, b, ab can be formally viewed as four colours, the permutation of which is defined by relations (3.4.3.14); then the group $\overline{\mathsf{J}}_{1j}$ can be treated as a four-colour layer group.

Since the symbol of a point group consists of generators from which any operation of the group can be derived by multiplication, one can derive from the international symbol of a sectional layer group, in which generators are supplied with adequate labels, the coset decomposition (3.4.4.13).

Thus for the domain pair $\{\mathbf{S}_1, \mathbf{S}_2\}$ in Fig. 3.4.4.2 with $J^\star_{12} = m^\star_x m_y m_z$ [see equation (3.4.3.18)] and $p(010)$ we get the sectional layer group $\overline{\mathsf{J}_{12}(010)} = m^\star_x\underline{m}_y m_z$. Operations of this group (besides generators) are $m^\star_x\underline{m}_y = \underline{2}^\star_z$, $\underline{m}_y m_z = \underline{2}_x$, $m^\star_x m_z = 2^\star_y$, $m^\star_x\underline{2}_x = \underline{\bar{1}}^\star$.

All operations $g \in G$ that transform a twin into itself constitute the *symmetry group* $\mathsf{T}_{1j}(\mathbf{n})$ (or in short T_{1j}) *of the twin* $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$. This is a layer group consisting of two parts:

$$\mathsf{T}_{1j} = \widehat{\mathsf{F}}_{1j} \cup \underline{t}^\star_{1j}\widehat{\mathsf{F}}_{1j}, \qquad (3.4.4.15)$$

where $\widehat{\mathsf{F}}_{1j}$ is a face group comprising all trivial symmetry operations of the twin and the left coset $\underline{t}^*_{1j}\widehat{\mathsf{F}}_{1j}$ contains all non-trivial operations of the twin that reverse the sides of the wall plane p and simultaneously exchange the states ($\mathbf{S}_1$ and $\mathbf{S}_j$).

One can easily verify that the symmetry $\mathsf{T}_{1j}(\mathbf{n})$ of the twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$ is equal to the symmetry $\mathsf{T}_{j1}(\mathbf{n})$ of the reversed twin $(\mathbf{S}_j|\mathbf{n}|\mathbf{S}_1)$,

$$\mathsf{T}_{1j}(\mathbf{n}) = \mathsf{T}_{j1}(\mathbf{n}). \qquad (3.4.4.16)$$

Similarly, for sectional layer groups,

$$\overline{\mathsf{F}}_{1j}(\mathbf{n}) = \overline{\mathsf{F}}_{j1}(\mathbf{n}) \ \text{and} \ \overline{\mathsf{J}}_{1j}(\mathbf{n}) = \overline{\mathsf{J}}_{j1}(\mathbf{n}). \qquad (3.4.4.17)$$

Table 3.4.4.3. *Classification of domain walls and simple twins*

T_{1j}	$\overline{\mathsf{J}}_{1j}$	Classification	Symbol
$\widehat{\mathsf{F}}_{1j} \cup \underline{t}^\star_{1j}\widehat{\mathsf{F}}_{1j}$	$\widehat{\mathsf{F}}_{1j} \cup \underline{t}^\star_{1j}\widehat{\mathsf{F}}_{1j} \cup r^\star_{1j}\widehat{\mathsf{F}}_{1j} \cup \underline{s}_{1j}\widehat{\mathsf{F}}_{1j}$	Symmetric reversible	SR
$\widehat{\mathsf{F}}_{1j} \cup \underline{t}^\star_{1j}\widehat{\mathsf{F}}_{1j}$	$\widehat{\mathsf{F}}_{1j} \cup \underline{t}^\star_{1j}\widehat{\mathsf{F}}_{1j}$	Symmetric irreversible	SI
$\widehat{\mathsf{F}}_{1j}$	$\widehat{\mathsf{F}}_{1j} \cup \underline{s}_{1j}\widehat{\mathsf{F}}_{1j}$	Asymmetric side-reversible	A$\underline{\mathrm{R}}$
$\widehat{\mathsf{F}}_{1j}$	$\widehat{\mathsf{F}}_{1j} \cup r^\star_{1j}\widehat{\mathsf{F}}_{1j}$	Asymmetric state-reversible	AR*
$\widehat{\mathsf{F}}_{1j}$	$\widehat{\mathsf{F}}_{1j}$	Asymmetric irreversible	AI

Therefore, the symmetry of a twin $\mathsf{T}_{1j}(p)$ and of sectional layer groups $\overline{\mathsf{F}}_{1j}(p)$, $\overline{\mathsf{J}}_{1j}(p)$ is specified by the orientation of the plane p [expressed *e.g.* by Miller indices (hkl)] and not by the sidedness of p. However, the two layer groups $\overline{\mathsf{F}}_{1j}(p)$ and $\overline{\mathsf{F}}_{j1}(p)$, and $\mathsf{T}_{1j}(p)$ and $\mathsf{T}_{j1}(p)$ express the symmetry of *two different* objects, which can in special cases (non-transposable pairs and irreversible twins) be symmetrically non-equivalent.

The symmetry $\mathsf{T}_{1j}(\mathbf{n})$ also expresses the symmetry of the wall $\mathbf{W}_{1j}(\mathbf{n})$. This symmetry imposes constraints on the form of tensors describing the properties of walls. In this way, the appearance of spontaneous polarization in domain walls has been examined (Přívratská & Janovec, 1999; Přívratská *et al.*, 2000).

According to their symmetry, twins and walls can be divided into two types: For a *symmetric twin (domain wall)*, there exists a non-trivial symmetry operation $\underline{t}^\star_{1j}$ and its symmetry is expressed by equation (3.4.4.15). A symmetric twin can be formed only from transposable domain pairs.

For an *asymmetric twin (domain wall)*, there is no non-trivial symmetry operation and its symmetry group is, therefore, confined to trivial group $\widehat{\mathsf{F}}_{1j}$,

$$\mathsf{T}_{1j} = \widehat{\mathsf{F}}_{1j}. \qquad (3.4.4.18)$$

The difference between symmetric and asymmetric walls can be visualized in domain walls of finite thickness treated in Section 3.4.4.6.

The symmetry T_{1j} of a symmetric twin (wall), expressed by relation (3.4.4.15), is a layer group but not a sectional layer group of any point group. It can, however, be derived from the sectional layer group $\overline{\mathsf{F}}_{1j}$ of the corresponding ordered domain pair $(\mathbf{S}_1, \mathbf{S}_j)$ [see equation (3.4.4.12)] and the sectional layer group $\overline{\mathsf{J}}_{1j}$ of the unordered domain pair $\{\mathbf{S}_1, \mathbf{S}_j\}$ [see equation (3.4.4.13)],

$$\mathsf{T}_{1j} = \overline{\mathsf{J}}_{1j} - \{\overline{\mathsf{F}}_{1j} - \widehat{\mathsf{F}}_{1j}\} - \{\widehat{\mathsf{J}}_{1j} - \widehat{\mathsf{F}}_{1j}\}. \qquad (3.4.4.19)$$

This is particularly useful in the microscopic description, since sectional layer groups of crystallographic planes in three-dimensional space groups are tabulated in *IT* E (2010), where one also finds an example of the derivation of the twin symmetry in the microscopic description.

The treatment of twin (wall) symmetry based on the concept of domain pairs and sectional layer groups of these pairs (Janovec, 1981; Zikmund, 1984) is analogous to the procedure used in treating interfaces in bicrystals (see Section 3.2.2; Pond & Bollmann, 1979; Pond & Vlachavas, 1983; Kalonji, 1985; Sutton & Balluffi, 1995). There is the following correspondence between terms: domain pair → dichromatic complex; domain wall → interface; domain twin with zero-thickness domain wall → ideal bicrystal; domain twin with finite-thickness domain wall → real (relaxed) bicrystal. Terms used in bicrystallography cover more general situations than domain structures (*e.g.* grain boundaries of crystals with non-crystallographic relations, phase interfaces). On the other hand, the existence of a high-symmetry phase, which is missing in bicrystallography, enables a more detailed discussion of crystallographically equivalent variants (orbits) of various objects in domain structures.

The symmetry group T_{1j} is the stabilizer of a domain twin (wall) in a certain group, and as such determines a class (orbit) of domain twins (walls) that are crystallographically equivalent with this twin (wall). The number of crystallographically equivalent twins is equal to the number of left cosets (index) of T_{1j} in the corresponding group. Thus the number $n_{W(p)}$ of equivalent domain twins (walls) with the same orientation defined by a plane p of the wall is

$$n_{W(p)} = [\overline{G(p)} : \mathsf{T}_{1j}] = |\overline{G(p)}| : |\mathsf{T}_{1j}|, \qquad (3.4.4.20)$$

where $\overline{G(p)}$ is a sectional layer group of the plane p in the parent group G, $[\overline{G(p)} : \mathsf{T}_{1j}]$ is the index of T_{1j} in $\overline{G(p)}$ and absolute value denotes the number of operations in a group.

The set of all domain walls (twins) crystallographically equivalent in G with a given wall $[\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j]$ forms a G-orbit of walls, $G\mathsf{W}_{1j} \equiv G[\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j]$. The number n_W of walls in this G-orbit is

$$\begin{aligned} n_W &= [G : \mathsf{T}_{1j}] = |G| : |\mathsf{T}_{1j}| = (|G| : |\overline{G(p)}|)(|\overline{G(p)}| : |\mathsf{T}_{1j}|) \\ &= n_p n_{W(p)}, \end{aligned} \qquad (3.4.4.21)$$

where n_p is the number of planes equivalent with plane p expressed by equation (3.4.4.9) and $n_{W(p)}$ is the number of equivalent domain walls with the plane p [see equation (3.4.4.20)]. Walls in one orbit have the same scalar properties (*e.g.* energy) and their structure and tensor properties are related by operations that relate walls from the same orbit.

Another aspect that characterizes twins and domain walls is the relation between a twin and the reversed twin. A twin (wall) which is crystallographically equivalent with the reversed twin (wall) will be called a *reversible twin (wall)*. If a twin and the reversed twin are not crystallographically equivalent, the twin will be called an *irreversible twin (wall)*. If a domain wall is reversible, then the properties of the reversed wall are fully specified by the properties of the initial wall, for example, these two walls have the same energy and their structures and properties are mutually related by a crystallographic operation. For irreversible walls, no relation exists between a wall and the reversed wall. Common examples of irreversible walls are electrically charged ferroelectric walls (walls carrying a nonzero polarization charge) and domain walls or discommensurations in phases with incommensurate structures.

A necessary and sufficient condition for reversibility is the existence of side-reversing and/or state-exchanging operations in the sectional layer group $\overline{\mathsf{J}}_{1j}$ of the unordered domain pair $\{\mathbf{S}_1, \mathbf{S}_j\}$ [see equation (3.4.4.13)]. This group also contains the symmetry group T_{1j} of the twin [see equation (3.4.4.15)] and thus provides a full symmetry characteristic of twins and walls,

$$\overline{\mathsf{J}}_{1j} = \mathsf{T}_{1j} \cup \underline{s}_{1j}\widehat{\mathsf{F}}_{1j} \cup \underline{t}^\star_{1j}\widehat{\mathsf{F}}_{1j}. \qquad (3.4.4.22)$$

Sequences of walls and reversed walls appear in simple lamellar domain structures which are formed by domains with two alternating domain states, say $\mathbf{S}_1$ and $\mathbf{S}_2$, and parallel walls W_{12} and reversed walls W_{21} (see Fig. 3.4.2.1).

The distinction 'symmetric–asymmetric' and 'reversible–irreversible' provides a natural classification of domain walls and simple twins. *Five prototypes of domain twins and domain walls*, listed in Table 3.4.4.3, correspond to five subgroups of the sectional layer group $\overline{\mathsf{J}}_{1j}$: the sectional layer group $\overline{\mathsf{J}}_{1j}$ itself, the layer group of the twin $\mathsf{T}_{1j} = \widehat{\mathsf{F}}_{1j} \cup \underline{t}^\star_{1j}\widehat{\mathsf{F}}_{1j}$, the sectional layer group

$\overline{\mathsf{F}}_{1j} = \widehat{\mathsf{F}}_{1j} \cup \underline{s}_{1j}\widehat{\mathsf{F}}_{1j}$, the trivial layer group $\widehat{\mathsf{J}}_{1j} = \widehat{\mathsf{F}}_{1j} \cup r^{*}_{1j}\widehat{\mathsf{F}}_{1j}$ and the trivial layer group $\widehat{\mathsf{F}}_{1j}$.

An example of a symmetric reversible (SR) twin (and wall) is the twin $(\mathbf{S}_1[010]\mathbf{S}_2)$ in Fig. 3.4.4.2 with a non-trivial twinning operation $\underline{2}^{\star}_{z}$ and with reversing operations $\underline{m}_y$ and $m^{\star}_{x}$. The twin $(\mathbf{S}_1^{+}[\bar{1}10]\mathbf{S}_3^{-})$ and reversed twin $(\mathbf{S}_3^{-}[\bar{1}10]\mathbf{S}_1^{+})$ in Fig. 3.4.3.8 are symmetric and irreversible (SI) twins with a twinning operation $\underline{m}^{\star}_{\bar{x}y}$; no reversing operations exist (walls are charged and charged walls are always irreversible, since a charge is invariant with respect to any transformation of the space). The twin $(\mathbf{S}_1^{-}[110]\mathbf{S}_3^{+})$ and reversed twin $(\mathbf{S}_3^{+}[110]\mathbf{S}_1^{-})$ in the same figure are asymmetric state-reversible twins with state-reversing operation $m^{\star}_{\bar{x}y}$ and with no non-trivial twinning operation.

The same classification also applies to domain twins and walls in a microscopic description.

As in the preceding section, we shall now present separately the symmetries of non-ferroelastic simple domain twins ['twinning without a change of crystal shape (or form)'] and of ferroelastic simple domain twins ['twinning with a change of crystal shape (or form)'; Klassen-Neklyudova (1964), Indenbom (1982)].

3.4.4.4. *Non-ferroelastic domain twins and domain walls*

Compatibility conditions impose no restriction on the orientation of non-ferroelastic domain walls. Any of the non-ferroelastic domain pairs listed in Table 3.4.3.4 can be sectioned on any crystallographic plane p and the sectional group $\overline{\mathsf{J}}_{1j}$ specifies the symmetry properties of the corresponding twin and domain wall. The analysis can be confined to one representative orientation of each class of equivalent planes, but a listing of all possible cases is too voluminous for the present article. We give, therefore, in Table 3.4.4.4 only possible symmetries T_{1j} and $\overline{\mathsf{J}}_{1j}$ of non-ferroelastic domain twins and walls, together with their classification, without specifying the orientation of the wall plane p.

Non-ferroelastic domain walls are usually curved with a slight preference for certain orientations (see Figs. 3.4.1.5 and 3.4.3.3). Such shapes indicate a weak anisotropy of the wall energy σ, *i.e.* small changes of σ with the orientation of the wall. The situation is different in ferroelectric domain structures, where charged domain walls have higher energies than uncharged ones.

A small energetic anisotropy of non-ferroelastic domain walls is utilized in producing *tailored domain structures* (Newnham *et al.*, 1975). A required domain pattern in a non-ferroelastic ferroelectric crystal can be obtained by evaporating electrodes of a desired shape (*e.g.* stripes) onto a single-domain plate cut perpendicular to the spontaneous polarization $\mathbf{P}_0$. Subsequent poling by an electric field switches only regions below the electrodes and thus produces the desired antiparallel domain structure.

Periodically poled ferroelectric domain structures fabricated by this technique are used for example in quasi-phase-matching optical multipliers (see *e.g.* Shur *et al.*, 1999, 2001; Rosenman *et al.*, 1998). An example of such an *engineered domain structure* is presented in Fig. 3.4.4.3.

Anisotropic domain walls can also appear if the Landau free energy contains a so-called Lifshitz invariant (see Section 3.1.3.3), which lowers the energy of walls with certain orientations and can be responsible for the appearance of an incommensurate phase (see *e.g.* Dolino, 1985; Tolédano & Tolédano, 1987; Tolédano & Dmitriev, 1996; Strukov & Levanyuk, 1998). The irreversible character of domain walls in a commensurate phase of crystals also containing (at least theoretically) an incommensurate phase has been confirmed in the frame of phenomenological theory by Ishibashi (1992). The incommensurate structure in quartz that demonstrates such an anisotropy is discussed at the end of the next example.

Table 3.4.4.4. *Symmetries of non-ferroelastic domain twins and walls*

T_{1j}	$\overline{\mathsf{J}}_{1j}$	Classification
1	1	AI
1	$\underline{\bar{1}}$	$\mathrm{A}\underline{\mathrm{R}}$
	$\underline{2}$	$\mathrm{A}\underline{\mathrm{R}}$
	$2^{\star}$	$\mathrm{AR}^{\star}$
	$m^{\star}$	$\mathrm{AR}^{\star}$
$\bar{1}^{\star}$	$\bar{1}^{\star}$	SI
	$\underline{2}/m^{\star}$	SR
	$2^{\star}/\underline{m}$	SR
2	$2m^{\star}m^{\star}$	$\mathrm{AR}^{\star}$
$\underline{2}^{\star}$	$\underline{2}^{\star}$	SI
	$\underline{2}^{\star}/m^{\star}$	SR
	$2^{\star}\underline{2}^{\star}\underline{2}$	SR
	$\underline{2}^{\star}\underline{m}m^{\star}$	SR
m	m	AI
	$\underline{2}/m$	$\mathrm{A}\underline{\mathrm{R}}$
	$2^{\star}mm^{\star}$	$\mathrm{AR}^{\star}$
$\underline{m}^{\star}$	$\underline{m}^{\star}$	SI
	$2^{\star}/\underline{m}^{\star}$	SR
	$\underline{m}^{\star}m^{\star}\underline{2}$	SR
$\underline{2}^{\star}/m$	$\underline{2}^{\star}/m$	SI
	$m\underline{m}m^{\star}$	SR
$2/\underline{m}^{\star}$	$2/\underline{m}^{\star}$	SI
	$m^{\star}m^{\star}\underline{m}^{\star}$	SR
	$4^{\star}/\underline{m}^{\star}$	SR
$2\underline{2}^{\star}\underline{2}^{\star}$	$2\underline{2}^{\star}\underline{2}^{\star}$	SI
	$\underline{m}m^{\star}m^{\star}$	SR
	$4^{\star}\underline{22}^{\star}$	SR
	$\underline{\bar{4}2}^{\star}m^{\star}$	SR
$\underline{m}^{\star}m\underline{2}^{\star}$	$\underline{m}^{\star}m\underline{2}^{\star}$	SI
	$\underline{m}^{\star}mm^{\star}$	SR
$mm\underline{m}^{\star}$	$mm\underline{m}^{\star}$	SI
	$4^{\star}/\underline{m}^{\star}m^{\star}m$	SR
4	$4m^{\star}m^{\star}$	$\mathrm{AR}^{\star}$
$\underline{\bar{4}}^{\star}$	$\underline{\bar{4}}^{\star}\underline{2}m^{\star}$	SR
$4/\underline{m}^{\star}$	$4/\underline{m}^{\star}$	SI
	$4/\underline{m}^{\star}m^{\star}m^{\star}$	SR
$4\underline{2}^{\star}\underline{2}^{\star}$	$4\underline{2}^{\star}\underline{2}^{\star}$	SI
	$4/\underline{m}m^{\star}m^{\star}$	SR
$\underline{\bar{4}}^{\star}\underline{2}^{\star}m$	$4^{\star}/\underline{m}m^{\star}m$	SR
$4/\underline{m}^{\star}mm$	$4/\underline{m}^{\star}mm$	SI
3	$3m^{\star}$	$\mathrm{AR}^{\star}$
	$6^{\star}$	$\mathrm{AR}^{\star}$
$\underline{\bar{3}}^{\star}$	$\underline{\bar{3}}^{\star}$	SI
	$\underline{\bar{3}}^{\star}m^{\star}$	SR
	$6^{\star}/\underline{m}$	SR
$3m$	$6^{\star}mm^{\star}$	$\mathrm{AR}^{\star}$
$3\underline{2}^{\star}$	$3\underline{2}^{\star}$	SI
	$\underline{\bar{3}}m^{\star}$	SR
	$6^{\star}\underline{22}^{\star}$	SR
	$\underline{\bar{6}2}^{\star}m^{\star}$	SR
$\underline{\bar{3}}^{\star}m$	$\underline{\bar{3}}^{\star}m$	SI
	$6^{\star}/\underline{m}mm^{\star}$	SR
6	$6m^{\star}m^{\star}$	$\mathrm{AR}^{\star}$
$\underline{\bar{6}}^{\star}$	$\underline{\bar{6}}^{\star}$	SI
	$6^{\star}/\underline{m}^{\star}$	SR
	$\underline{\bar{6}}^{\star}\underline{2}m^{\star}$	SR
$6/\underline{m}^{\star}$	$6/\underline{m}^{\star}$	SI
	$6/\underline{m}^{\star}m^{\star}m^{\star}$	SR
$6\underline{2}^{\star}\underline{2}^{\star}$	$6\underline{2}^{\star}\underline{2}^{\star}$	SI
	$6/\underline{m}m^{\star}m^{\star}$	SR
$\underline{\bar{6}}^{\star}m\underline{2}^{\star}$	$\underline{\bar{6}}^{\star}m\underline{2}^{\star}$	SI
	$6^{\star}/\underline{m}^{\star}mm^{\star}$	SR
$6/\underline{m}^{\star}mm$	$6/\underline{m}^{\star}mm$	SI

references