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

T_{1j}	$\overline{\mathsf{J}}_{1j}$	Classification	Symbol
$\widehat{\mathsf{F}}_{1j} \cup \underline{t}^{*}_{1j}\widehat{\mathsf{F}}_{1j}$	$\widehat{\mathsf{F}}_{1j} \cup \underline{t}^{*}_{1j}\widehat{\mathsf{F}}_{1j} \cup r^{*}_{1j}\widehat{\mathsf{F}}_{1j} \cup \underline{s}_{1j}\widehat{\mathsf{F}}_{1j}$	Symmetric reversible	SR
$\widehat{\mathsf{F}}_{1j} \cup \underline{t}^{*}_{1j}\widehat{\mathsf{F}}_{1j}$	$\widehat{\mathsf{F}}_{1j} \cup \underline{t}^{*}_{1j}\widehat{\mathsf{F}}_{1j}$	Symmetric irreversible	SI
$\widehat{\mathsf{F}}_{1j}$	$\widehat{\mathsf{F}}_{1j} \cup \underline{s}_{1j}\widehat{\mathsf{F}}_{1j}$	Asymmetric side-reversible	A$\underline{\text{R}}$
$\widehat{\mathsf{F}}_{1j}$	$\widehat{\mathsf{F}}_{1j} \cup r^{*}_{1j}\widehat{\mathsf{F}}_{1j}$	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 $\mathsf{T}_{1j} = \widehat{\mathsf{F}}_{1j} \cup \underline{t}^{*}_{1j}\widehat{\mathsf{F}}_{1j}$, the sectional layer group

references