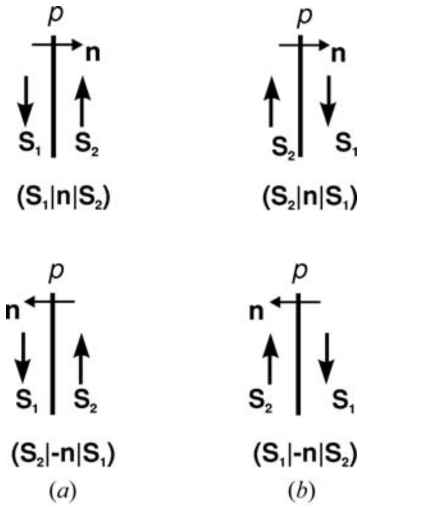

Fig. 3.4.4.1. Symbols of a simple twin. (*a*) Two different symbols with antiparallel normal **n**. (*b*) Symbols of the reversed twin.

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)

Copyright © 2013 International Union of Crystallography