

3. SYMMETRY ASPECTS OF PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

Table 3.4.4.1. Crystallographic layer groups with continuous translations

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

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

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).

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

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 ($S_1 | \mathbf{n} | S_j$) 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 W_{ij} 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 ($S_1 | \mathbf{n} | S_j$), we get a crystallographically equivalent twin ($S_i | \mathbf{n}_m | S_k$) $\overset{G}{\sim}$ ($S_1 | \mathbf{n} | S_j$) with other domain states and another orientation of the domain wall,

$$g(S_1 | \mathbf{n} | S_j) = (gS_1 | g\mathbf{n} | gS_j) = (S_i | \mathbf{n}_m | S_k), \quad g \in G. \quad (3.4.4.11)$$

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 GS_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 ($S_1 | \mathbf{n} | S_j$) 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 S_1 and 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 ($S_1 | [010] | S_2$) with domain states S_1 and S_2 from our illustrative example (see Fig. 3.4.2.2).

(1) An operation f_{ij} which leaves invariant the normal \mathbf{n} and both domain states S_1, S_j in the twin ($S_1 | \mathbf{n} | S_j$); 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 ($S_1 | [010] | S_2$) in Fig. 3.4.4.2 is the reflection m_z .

(2) An operation \underline{s}_{ij} which inverts the normal \mathbf{n} but leaves invariant both domain states S_1 and S_j . This *side-reversing operation* transforms the initial twin ($S_1 | \mathbf{n} | S_j$) into ($S_1 | -\mathbf{n} | S_j$), which is, according to (3.4.4.1), identical with the inverse twin ($S_j | \mathbf{n} | S_1$). 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_{ij}^* which exchanges domain states S_1 and S_j but does not change the normal \mathbf{n} . This *state-exchanging operation*, denoted by a star symbol, transforms the initial twin ($S_1 | \mathbf{n} | S_j$) into a reversed twin ($S_j | \mathbf{n} | S_1$). A state-exchanging operation in our example is the reflection m_x^* .

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 $\bar{1}$ 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 & Kopicik (1974).

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

$$\overline{G(p)} = \widehat{G(p)} \cup \underline{\widehat{G(p)}}, \quad (3.4.4.8)$$

where the trivial layer group $\widehat{G(p)}$ 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 $\underline{\widehat{G(p)}}$ contains all side-reversing operations of $\overline{G(p)}$.

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