

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

Table 3.4.3.3. Decomposition of  $G = 6_z/m_z$  into left cosets of  $F_1 = 2_z/m_z$

| Left coset |         |               |               | Principal domain state |
|------------|---------|---------------|---------------|------------------------|
| 1          | $2_z$   | $\bar{1}$     | $m_z$         | $S_1$                  |
| $3_z$      | $6_z^5$ | $\bar{3}_z$   | $\bar{6}_z^5$ | $S_2$                  |
| $3_z^2$    | $6_z$   | $\bar{3}_z^5$ | $\bar{6}_z$   | $S_3$                  |

of this double coset belongs to this double coset, hence it is a multiple invertible double coset. Corresponding domain pairs are partially transposable ones. A representative pair is, for example,  $(S_1, 2_{xy}S_1) = (S_1, S_3)$  which is indeed a partially transposable domain pair [cf. (3.4.3.19) and (3.4.3.20)]. The class of equivalent ordered domain pairs is  $(S_1, S_3) \stackrel{G}{\sim} (S_3, S_1) \stackrel{G}{\sim} (S_1, S_4) \stackrel{G}{\sim} (S_4, S_1) \stackrel{G}{\sim} (S_3, S_2) \stackrel{G}{\sim} (S_2, S_3) \stackrel{G}{\sim} (S_2, S_4) \stackrel{G}{\sim} (S_4, S_2)$ . These are ‘90° domain pairs’.

An example of non-invertible double cosets is provided by the decomposition of the group  $G = 6_z/m_z$  into left and double cosets of  $F_1 = 2_z/m_z$  displayed in Table 3.4.3.3. The inverse of the second left coset (second line) is equal to the third left coset (third line) and vice versa. Each of these two left cosets thus corresponds to a double coset and these double cosets are complementary double cosets. Corresponding representative simple non-transposable domain pairs are  $(S_1, S_2)$  and  $(S_2, S_1)$ , and are depicted in Fig. 3.4.3.2.

We conclude that double cosets determine classes of equivalent domain pairs that can appear in the ferroic phase resulting from a phase transition with a symmetry descent  $G \supset F_1$ . Left coset and double coset decompositions for all crystallographic point-group descents are available in the software *GI★KoBo-1*, path: *Subgroups\View\Twinning groups*.

A double coset can be specified by any operation belonging to it. This representation is not very convenient, since it does not reflect the properties of corresponding domain pairs and there are many operations that can be chosen as representatives of a double coset. It turns out that in a continuum description the twinning group  $K_{ij}$  can represent classes of equivalent domain pairs  $G(S_1, S_j)$  with two exceptions:

(i) Two complementary classes of non-transposable domain pairs have the same twinning group. This follows from the fact that if a twinning group contains the double coset, then it must comprise also the inverse double coset.

(ii) Different classes of transposable domain pairs have different twinning groups except in the following case (which corresponds to the orthorhombic ferroelectric phase in perovskites): the group  $F_1 = m_{xy}2_{xy}m_z$  generates with switching operations  $g = 2_{yz}$  and  $g_3 = m_{yz}$  two different double cosets with the same twinning group  $K_{12} = K_{13} = m\bar{3}m$  (one can verify this in the software *GI★KoBo-1*, path: *Subgroups\View\Twinning groups*). Domain states are characterized in this ferroelectric phase by the direction of the spontaneous polarization. The angles between the spontaneous polarizations of the domain states in domain pairs  $(S_1, 2_{yz}S_1)$  and  $(S_1, m_{yz}S_1)$  are 120 and 60°, respectively; this shows that these representative domain pairs are not equivalent and belong to two different  $G$ -orbits of domain pairs. To distinguish these two cases, we add to the twinning group  $m\bar{3}m[m_{xy}2_{xy}m_z]$  either the switching operation  $2_{yz}$  or  $m_{yz}$ , i.e. the two distinct orbits are labelled by the symbols  $m\bar{3}m(2_{xy})$  and  $m\bar{3}m(m_{xy})$ , respectively.

Bearing in mind these two exceptions, one can, in the continuum description, represent  $G$ -orbits of domain pairs  $G(S_1, S_j)$  by twinning groups  $K_{ij}(F_1)$ .

We have used this correspondence in synoptic Table 3.4.2.7 of symmetry descents at ferroic phase transitions. For each symmetry descent  $G \supset F_1$ , the twinning groups given in column  $K_{ij}$  specify possible  $G$ -orbits of domain pairs that can appear in the domain structure of the ferroic phase (Litvin & Janovec, 1999).

We divide all orbits of domain pairs (represented by corresponding twinning groups  $K_{ij}$ ) that appear in Table 3.4.2.7 into classes of non-ferroelastic and ferroelastic domain pairs and present them with further details in the three synoptic Tables 3.4.3.4, 3.4.3.6 and 3.4.3.7 described in Sections 3.4.3.5 and 3.4.3.6.

As we have seen, a classification of domain pairs according to their internal symmetry (summarized in Table 3.4.3.2) introduces a partition of all domain pairs that can be formed from domain states of the  $G$ -orbit  $GS_1$  into equivalence classes of pairs with the same internal symmetry. Similarly, any inherent physical property of domain pairs induces a partition of all domain pairs into corresponding equivalence classes. Thus, for example, the classification of domain pairs, based on tensor distinction or switching of domain states (see Table 3.4.3.1, columns two and three), introduces a division of domain pairs into corresponding equivalence classes.

3.4.3.5. Non-ferroelastic domain pairs: twin laws, domain distinction and switching fields, synoptic table

Two domain states  $S_1$  and  $S_j$  form a non-ferroelastic domain pair  $(S_1, S_j)$  if the spontaneous strain in both domain states is the same,  $u_0^{(1)} = u_0^{(j)}$ . This is so if the twinning group  $K_{ij}$  of the pair and the symmetry group  $F_1$  of domain state  $S_1$  belong to the same crystal family (see Table 3.4.2.2):

$$\text{Fam}K_{ij} = \text{Fam}F_1. \tag{3.4.3.40}$$

It can be shown that all non-ferroelastic domain pairs are completely transposable domain pairs (Janovec et al., 1993), i.e.

$$F_{ij} = F_1 = F_j \tag{3.4.3.41}$$

and the twinning group  $K_{ij}$  is equal to the symmetry group  $J_{ij}$  of the unordered domain pair [see equation (3.4.3.24)]:

$$K_{ij}^* = J_{ij}^* = F_1 \cup g_{ij}^*F_1. \tag{3.4.3.42}$$

(Complete transposability is only a necessary, but not a sufficient, condition of a non-ferroelastic domain pair, since there are also ferroelastic domain pairs that are completely transposable – see Table 3.4.3.6.)

The relation between domain states in a non-ferroelastic domain twin, in which two domain states coexist, is the same as that of a corresponding non-ferroelastic domain pair consisting of single-domain states. Transposing operations  $g_{ij}^*$  are, therefore, also twinning operations.

Synoptic Table 3.4.3.4 lists representative domain pairs of all orbits of non-ferroelastic domain pairs. Each pair is specified by the first domain state  $S_1$  with symmetry group  $F_1$  and by transposing operations  $g_{ij}^*$  that transform  $S_1$  into  $S_j$ ,  $S_j = g_{ij}^*S_1$ . Twin laws in dichromatic notation are presented and basic data for tensor distinction and switching of non-ferroelastic domains are given.

3.4.3.5.1. Explanation of Table 3.4.3.4

The first three columns specify domain pairs.

$F_1$ : point-group symmetry (stabilizer in  $K_{ij}$ ) of the first domain state  $S_1$  in a single-domain orientation. There are two domain states with the same  $F_1$ ; one has to be chosen as  $S_1$ . Subscripts of generators in the group symbol specify their orientation in the Cartesian (rectangular) crystallophysical coordinate system of the group  $K_{ij}$  (see Tables 3.4.2.5, 3.4.2.6 and Figs. 3.4.2.3, 3.4.2.4).

$g_{ij}^*$ : switching operations that specify domain pair  $(S_1, g_{ij}^*S_1) = (S_1, S_j)$ . Subscripts of symmetry operations specify the orientation of the corresponding symmetry element in the Cartesian (rectangular) crystallophysical coordinate system of the group  $K_{ij}$ . In hexagonal and trigonal systems,  $x'$ ,  $y'$  and  $x''$ ,  $y''$  denote the Cartesian coordinate system rotated about the  $z$  axis through 120 and 240°, respectively, from the Cartesian coordinate axes  $x$