International Tables for Crystallography (2013). Vol. D, Section 3.4.3.4, pp. 511–512.

Table 3.4.3.2. *Four types of domain pairs*

F_{1j}	J_{1j}	K_{1j}	Double coset	Domain pair name symbol	
$F_1 = F_j$	$F_1 \cup g^\star_{1j}F_1$	$F_1 \cup g^\star_{1j}F_1$	$F_1g_{1j}F_1 = g_{1j}F_1 = (g_{1j}F_1)^{-1}$	transposable completely	tc
$F_{1j} \subset F_1$	$F_{1j} \cup g^\star_{1j}F_{1j}$	$F_1 \cup g^\star_{1j}F_1 \cup \ldots$	$F_1g_{1j}F_1 = (F_1g_{1j}F_1)^{-1}$	transposable partially	tp
$F_1 = F_j$	F_1	$F_1 \cup g_{1j}F_1 \cup g^{-1}_{1j}F_1$	$F_1g_{1j}F_1 = g_{1j}F_1 \cap (g_{1j}F_1)^{-1} = \emptyset$	non-transposable simple	ns
$F_{1j} \subset F_1$	F_{1j}	$F_1 \cup g_{1j}F_1 \cup (g_{1j}F_1)^{-1} \cup \ldots$	$F_1g_{1j}F_1 \cap (F_1g_{1j}F_1)^{-1} = \emptyset$	non-transposable multiple	nm

(Wadhawan, 2000). We consider in our classification always the potential ferroelectric (ferroelastic) phase.

A closer look at equation (3.4.3.33) reveals a correspondence between the difference coefficients in front of products of field components and the tensor distinction of domain states $\mathbf{S}_1$ and $\mathbf{S}_j$ in the domain pair $(\mathbf{S}_1, \mathbf{S}_j)$: If a morphic Cartesian tensor component of a *polar* tensor is different in these two domain states, then the corresponding difference coefficient is nonzero and defines components of fields that can switch one of these domain states into the other. A similar statement holds for the symmetric tensors of rank two (*e.g.* the spontaneous strain tensor).

Tensor distinction for all representative non-ferroelastic domain pairs is available in the synoptic Table 3.4.3.4. These data also carry information about the switching fields.

3.4.3.4. *Classes of equivalent domain pairs and their classifications*

Two domain pairs that are crystallographically equivalent, $(\mathbf{S}_i, \mathbf{S}_k) \overset{G}{\sim} (\mathbf{S}_l, \mathbf{S}_m)$ [see equation (3.4.3.5)], have different orientations in space but their inherent properties are the same. It is, therefore, useful to divide all domain pairs of a ferroic phase into classes of equivalent domain pairs. All domain pairs that are equivalent (in G) with a given domain pair, say $(\mathbf{S}_i, \mathbf{S}_k)$, can be obtained by applying to $(\mathbf{S}_i, \mathbf{S}_k)$ all operations of G, *i.e.* by forming a G-orbit $G(\mathbf{S}_i, \mathbf{S}_k)$.

One can always find in this orbit a domain pair $(\mathbf{S}_1, \mathbf{S}_j)$ that has in the first place the first domain state $\mathbf{S}_1$. We shall call such a pair a *representative domain pair of the orbit*. The initial orbit $G(\mathbf{S}_i, \mathbf{S}_k)$ and the orbit $G(\mathbf{S}_1, \mathbf{S}_j)$ are identical:

$$G(\mathbf{S}_i, \mathbf{S}_k) = G(\mathbf{S}_1, \mathbf{S}_j).$$

The set P of n^2 ordered pairs (including trivial ones) that can be formed from n domain states can be divided into G-orbits (classes of equivalent domain pairs):

$$\mathsf{P} = G(\mathbf{S}_1, \mathbf{S}_1) \cup G(\mathbf{S}_1, g_2\mathbf{S}_1) \cup \ldots \cup (\mathbf{S}_1, g_j\mathbf{S}_1) \cup \ldots \cup G(\mathbf{S}_1, g_q\mathbf{S}_1). \quad (3.4.3.34)$$

Similarly, as there is a one-to-one correspondence between domain states and left cosets of the stabilizer (symmetry group) F_1 of the first domain state [see equation (3.4.2.9)], there is an analogous relation between G-orbits of domain pairs and so-called double cosets of F_1.

A *double coset* $F_1g_jF_1$ *of* F_1 is a set of left cosets that can be expressed as fg_jF_1, where $f \in F_1$ runs over all operations of F_1 (see Section 3.2.3.2.8). A group G can be decomposed into disjoint double cosets of $F_1 \subset G$:

$$G = F_1eF_1 \cup F_1g_2F_1 \cup \ldots \cup F_1g_jF_1 \cup \ldots \cup F_1g_qF_1, \quad j = 1, 2, \ldots, q, \quad (3.4.3.35)$$

where $g_1 = e, g_2, \ldots g_j, \ldots g_q$ is the set of representatives of double cosets.

There is a one-to-one correspondence between double cosets of the decomposition (3.4.3.35) and G-orbits of domain pairs (3.4.3.34) (see Section 3.2.3.3.6, Proposition 3.2.3.35):

$$G(\mathbf{S}_1, \mathbf{S}_j) \leftrightarrow F_1g_jF_1, \quad \text{where} \quad \mathbf{S}_j = g_j\mathbf{S}_1, \quad j = 1, 2, \ldots, q. \quad (3.4.3.36)$$

We see that the representatives g_j of the double cosets in decomposition (3.4.3.35) define domain pairs $(\mathbf{S}_1, g_j\mathbf{S}_1)$ which represent all different G-orbits of domain pairs. Just as different left cosets g_iF_1 specify all domain states, different double cosets determine all classes of equivalent domain pairs (G-orbits of domain pairs).

The properties of double cosets are reflected in the properties of corresponding domain pairs and provide a natural classification of domain pairs. A specific property of a double coset is that it is either identical or disjoint with its inverse. A double coset that is identical with its inverse,

$$(F_1g_jF_1)^{-1} = F_1g_j^{-1}F_1 = F_1g_jF_1, \quad (3.4.3.37)$$

is called an *invertible (ambivalent) double coset*. The corresponding class of domain pairs consists of transposable (ambivalent) domain pairs.

A double coset that is disjoint with its inverse,

$$(F_1g_jF_1)^{-1} = F_1g_j^{-1}F_1 \cap F_1g_jF_1 = \emptyset, \quad (3.4.3.38)$$

is a *non-invertible (polar) double coset* ($\emptyset$ denotes an empty set) and the corresponding class of domain pairs comprises non-transposable (polar) domain pairs. A double coset $F_1g_jF_1$ and its inverse $(F_1g_jF_1)^{-1}$ are called *complementary double cosets*. Corresponding classes called *complementary classes of equivalent domain pairs* consist of transposed domain pairs that are non-equivalent.

Another attribute of a double coset is the number of left cosets which it comprises. If an invertible double coset consists of one left coset,

$$F_1g_jF_1 = g_jF_1 = (g_jF_1)^{-1}, \quad (3.4.3.39)$$

then the domain pairs in the G-orbit $G(\mathbf{S}_1, g_j\mathbf{S}_1)$ are completely transposable. An invertible double coset comprising several left cosets is associated with a G-orbit consisting of partially transposable domain pairs. Non-invertible double cosets can be divided into simple non-transposable double cosets (complementary double cosets consist of one left coset each) and multiple non-transposable double cosets (complementary double cosets comprise more than one left coset each).

Thus there are four types of double cosets (see Table 3.2.3.1 in Section 3.2.3.2) to which there correspond the four basic types of domain pairs presented in Table 3.4.3.2.

These results can be illustrated using the example of a phase transition with $G = 4_z/m_zm_xm_{xy} \supset 2_xm_ym_z = F_1$ with four domain states (see Fig. 3.4.2.2). The corresponding four left cosets of $2_xm_ym_z$ are given in Table 3.4.2.1. Any operation from the first left coset (identical with F_1) transforms the second left coset into itself, *i.e.* this left coset is a double coset. Since it consists of an operation of order two, it is a simple invertible double coset. The corresponding representative domain pair is $(\mathbf{S}_1, \bar{1}\mathbf{S}_1) = (\mathbf{S}_1, \mathbf{S}_2)$. By applying operations of $G = 4_z/m_zm_xm_{xy}$ on $(\mathbf{S}_1, \mathbf{S}_2)$, one gets the class of equivalent domain pairs (G-orbit): $(\mathbf{S}_1, \mathbf{S}_2) \overset{G}{\sim} (\mathbf{S}_2, \mathbf{S}_1) \overset{G}{\sim} (\mathbf{S}_3, \mathbf{S}_4) \overset{G}{\sim} (\mathbf{S}_4, \mathbf{S}_3)$. These domain pairs can be labelled as '180° pairs' according to the angle between the spontaneous polarization in the two domain states.

When one applies operations from the first left coset on the third left coset, one gets the fourth left coset, therefore a double coset consists of these two left cosets. An inverse of any operation

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	$\mathbf{S}_1$
3_z	6_z^5	$\bar{3}_z$	$\bar{6}_z^5$	$\mathbf{S}_2$
3_z^2	6_z	$\bar{3}_z^5$	$\bar{6}_z$	$\mathbf{S}_3$

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, $(\mathbf{S}_1, 2_{xy}\mathbf{S}_1) = (\mathbf{S}_1, \mathbf{S}_3)$ 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 $(\mathbf{S}_1, \mathbf{S}_3) \overset{G}{\sim} (\mathbf{S}_3, \mathbf{S}_1) \overset{G}{\sim} (\mathbf{S}_1, \mathbf{S}_4) \overset{G}{\sim} (\mathbf{S}_4, \mathbf{S}_1) \overset{G}{\sim} (\mathbf{S}_3, \mathbf{S}_2) \overset{G}{\sim} (\mathbf{S}_2, \mathbf{S}_3) \overset{G}{\sim} (\mathbf{S}_2, \mathbf{S}_4) \overset{G}{\sim} (\mathbf{S}_4, \mathbf{S}_2)$. 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 $(\mathbf{S}_1, \mathbf{S}_2)$ and $(\mathbf{S}_2, \mathbf{S}_1)$, 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_{1j} can represent classes of equivalent domain pairs $G(\mathbf{S}_1, \mathbf{S}_j)$ 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 twining groups except in the following case (which corresponds to the orthorhombic ferroelectric phase in perovskites): the group $F_1 = m_{x\bar{y}}2_{xy}m_z$ 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 $(\mathbf{S}_1, 2_{yz}\mathbf{S}_1)$ and $(\mathbf{S}_1, m_{yz}\mathbf{S}_1)$ 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 $m\bar{3}m[m_{x\bar{y}}2_{xy}m_z]$ 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 $G(\mathbf{S}_1, \mathbf{S}_j)$ by twinning groups $K_{1j}(F_1)$.*

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_{1j} 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_{1j}) 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 $G\mathbf{S}_1$ 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 $\mathbf{S}_1$ and $\mathbf{S}_j$ form a *non-ferroelastic domain pair* $(\mathbf{S}_1, \mathbf{S}_j)$ if the spontaneous strain in both domain states is the same, $\mathbf{u}_0^{(1)} = \mathbf{u}_0^{(j)}$. This is so if the twinning group K_{1j} of the pair and the symmetry group F_1 of domain state $\mathbf{S}_1$ belong to the same crystal family (see Table 3.4.2.2):

$$\mathrm{Fam}K_{1j} = \mathrm{Fam}F_1. \qquad (3.4.3.40)$$

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

$$F_{1j} = F_1 = F_j \qquad (3.4.3.41)$$

and the twinning group K_{1j} is equal to the symmetry group J_{1j} of the unordered domain pair [see equation (3.4.3.24)]:

$$K_{1j}^\star = J_{1j}^\star = F_1 \cup g_{1j}^\star F_1. \qquad (3.4.3.42)$$

(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 $g_{1j}^\star$ 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 $\mathbf{S}_1$ with symmetry group F_1 and by transposing operations $g_{1j}^\star$ that transform $\mathbf{S}_1$ into $\mathbf{S}_j$, $\mathbf{S}_j = g_{1j}^\star\mathbf{S}_1$. 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_{1j}) of the first domain state $\mathbf{S}_1$) in a single-domain orientation*. There are two domain states with the same F_1; one has to be chosen as $\mathbf{S}_1$. Subscripts of generators in the group symbol specify their orientation in the Cartesian (rectangular) crystallophysical coordinate system of the group K_{1j} (see Tables 3.4.2.5, 3.4.2.6 and Figs. 3.4.2.3, 3.4.2.4).

$g_{1j}^\star$: *switching operations* that specify domain pair $(\mathbf{S}_1, g_{1j}^\star\mathbf{S}_1) = (\mathbf{S}_1, \mathbf{S}_j)$. Subscripts of symmetry operations specify the orientation of the corresponding symmetry element in the Cartesian (rectangular) crystallophysical coordinate system of the group K_{1j}. 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