

3.4. DOMAIN STRUCTURES

Table 3.4.3.2. Four types of domain pairs

F_{ij}	J_{ij}	K_{ij}	Double coset	Domain pair name symbol
$F_i = F_j$	$F_i \cup g_{ij}^* F_i$	$F_i \cup g_{ij}^* F_i$	$F_i g_{ij} F_i = g_{ij} F_i = (g_{ij} F_i)^{-1}$	<u>t</u> ransposable <u>c</u> ompletely tc
$F_{ij} \subset F_i$	$F_{ij} \cup g_{ij}^* F_{ij}$	$F_i \cup g_{ij}^* F_i \cup \dots$	$F_i g_{ij} F_i = (F_i g_{ij} F_i)^{-1}$	<u>t</u> ransposable <u>p</u> artially tp
$F_i = F_j$	F_i	$F_i \cup g_{ij} F_i \cup g_{ij}^{-1} F_i$	$F_i g_{ij} F_i = g_{ij} F_i \cap (g_{ij} F_i)^{-1} = \emptyset$	<u>n</u> on-transposable <u>s</u> imple ns
$F_{ij} \subset F_i$	F_{ij}	$F_i \cup g_{ij} F_i \cup (g_{ij} F_i)^{-1} \cup \dots$	$F_i g_{ij} F_i \cap (F_i g_{ij} F_i)^{-1} = \emptyset$	<u>n</u> on-transposable <u>m</u> ultiple 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}_i and \mathbf{S}_j in the domain pair $(\mathbf{S}_i, \mathbf{S}_j)$: 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, $(\mathbf{S}_i, \mathbf{S}_k) \stackrel{G}{\sim} (\mathbf{S}_l, \mathbf{S}_m)$ [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 $(\mathbf{S}_i, \mathbf{S}_j)$ that has in the first place the first domain state \mathbf{S}_i . 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 $G(\mathbf{S}_i, \mathbf{S}_j)$ are identical:

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

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):

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

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* $F_i g_j F_1$ of F_1 is a set of left cosets that can be expressed as $f g_j F_1$, 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 $F_1 \subset G$:

$$G = F_1 e F_1 \cup F_1 g_2 F_1 \cup \dots \cup F_1 g_j F_1 \cup \dots \cup F_1 g_q F_1, \quad j = 1, 2, \dots, q, \quad (3.4.3.35)$$

where $g_1 = e, g_2, \dots, g_j, \dots, g_q$ 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 3.2.3.3.5):

$$G(\mathbf{S}_i, \mathbf{S}_j) \leftrightarrow F_i g_j F_1, \quad \text{where } \mathbf{S}_j = g_j \mathbf{S}_i, \quad j = 1, 2, \dots, q. \quad (3.4.3.36)$$

We see that the representatives g_j of the double cosets in decomposition (3.4.3.35) define domain pairs $(\mathbf{S}_i, g_j \mathbf{S}_i)$ which represent all different G -orbits of domain pairs. Just as different left cosets $g_i F_1$ 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,

$$(F_i g_j F_1)^{-1} = F_i g_j^{-1} F_1 = F_i g_j F_1, \quad (3.4.3.37)$$

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,

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

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 $F_i g_j F_1$ and its inverse $(F_i g_j F_1)^{-1}$ 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,

$$F_i g_j F_1 = g_j F_1 = (g_j F_1)^{-1}, \quad (3.4.3.39)$$

then the domain pairs in the G -orbit $G(\mathbf{S}_i, g_j \mathbf{S}_i)$ 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 $G = 4_z/m_z m_x m_{xy} \supset 2_x m_y m_z = F_1$ with four domain states (see Fig. 3.4.2.2). The corresponding four left cosets of $2_x m_y m_z$ 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 $G = 4_z/m_z m_x m_{xy}$ on $(\mathbf{S}_1, \mathbf{S}_2)$, one gets the class of equivalent domain pairs (G -orbit): $(\mathbf{S}_1, \mathbf{S}_2) \stackrel{G}{\sim} (\mathbf{S}_2, \mathbf{S}_1) \stackrel{G}{\sim} (\mathbf{S}_3, \mathbf{S}_4) \stackrel{G}{\sim} (\mathbf{S}_4, \mathbf{S}_3)$. 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