

3.4. DOMAIN STRUCTURES

domain states differ in principal tensor parameters (these are linear combinations of morphic tensor components that transform as the primary order parameter of an equitranslational phase transition with a point-group symmetry descent $G \supset F_1$, see Sections 3.1.3.2 and 3.4.2.3). A simple criterion for a principal domain state \mathbf{S}_1 is that its stabilizer in G is equal to the symmetry F_1 of the ferroic phase [see equation (3.4.2.4)].

When one applies to a principal domain state \mathbf{S}_1 all operations of the group G , one gets all principal domain states that are crystallographically equivalent with \mathbf{S}_1 . The set of all these states is denoted $G\mathbf{S}_1$ and is called an G -orbit of \mathbf{S}_1 (see also Section 3.2.3.3.3),

$$G\mathbf{S}_1 = \{\mathbf{S}_1, \mathbf{S}_2, \dots, \mathbf{S}_n\}. \quad (3.4.2.6)$$

In our example, the G -orbit is $4_z/m_z m_x m_{xy} \mathbf{S}_1 = \{\mathbf{S}_1, \mathbf{S}_2, \mathbf{S}_3, \mathbf{S}_4\}$.

Note that any operation g from the parent group G leaves the orbit $G\mathbf{S}_1$ invariant since its action results only in a permutation of all principal domain states. This change does not alter the orbit, since the orbit is a set in which the sequence (order) of objects is irrelevant. Therefore, the orbit $G\mathbf{S}_1$ is invariant under the action of the parent group G , $G(G\mathbf{S}_1) = G\mathbf{S}_1$.

A ferroic phase transition is thus a paradigmatic example of the law of symmetry compensation (see Section 3.2.2): The dissymmetrization of a high-symmetry parent phase into a low-symmetry ferroic phase produces variants of the low-symmetry ferroic phase (single-domain states). Any two single-domain states are related by some suppressed operations of the parent symmetry that are missing in the ferroic symmetry and the set of all single-domain states (G -orbit of domain states) recovers the symmetry of the parent phase. If the domain structure contains all domain states with equal partial volumes then the average symmetry of this polydomain structure is, in the first approximation, identical to the symmetry of the parent phase.

Now we find a simple formula for the number n of principal domain states in the orbit $G\mathbf{S}_1$ and a recipe for an efficient generation of all principal domain states in this orbit.

The fact that all operations of the group $I_G(\mathbf{S}_1) = F_1$ leave \mathbf{S}_1 invariant can be expressed in an abbreviated form in the following way [see equation (3.2.3.70)]:

$$F_1 \mathbf{S}_1 = \mathbf{S}_1. \quad (3.4.2.7)$$

We shall use this relation to derive all operations that transform \mathbf{S}_1 into $\mathbf{S}_j = g_j \mathbf{S}_1$:

$$g_j \mathbf{S}_1 = g_j (F_1 \mathbf{S}_1) = (g_j F_1) \mathbf{S}_1 = \mathbf{S}_j, \quad g_j \in G. \quad (3.4.2.8)$$

The second part of equation (3.4.2.8) shows that all lost operations that transform \mathbf{S}_1 into \mathbf{S}_j are contained in the left coset $g_j F_1$ (for left cosets see Section 3.2.3.2.3).

It is shown in group theory that two left cosets have no operation in common. Therefore, another left coset $g_k F_1$ generates another principal domain state \mathbf{S}_k that is different from principal domain states \mathbf{S}_1 and \mathbf{S}_j . Equation (3.4.2.8) defines, therefore, a one-to-one relation between principal domain states of the orbit $G\mathbf{S}_1$ and left cosets of F_1 [see equation (3.2.3.69)],

$$\mathbf{S}_j \leftrightarrow g_j F_1, \quad F_1 = I_G(\mathbf{S}_1), \quad j = 1, 2, \dots, n. \quad (3.4.2.9)$$

From this relation follow two conclusions:

(1) The number n of principal domain states equals the number of left cosets of F_1 . All different left cosets of F_1 constitute the decomposition of the group G into left cosets of F_1 [see equation (3.2.3.19)],

$$G = g_1 F_1 \cup g_2 F_1 \cup \dots \cup g_j F_1 \cup \dots \cup g_n F_1, \quad (3.4.2.10)$$

where the symbol \cup is a union of sets and the number n of left cosets is called the index of G in F_1 and is denoted by the symbol $[G : F_1]$. Usually, one chooses for g_1 the identity operation e ; then the first left coset equals F_1 . Since each left coset contains $|F_1|$ operations, where $|F_1|$ is number of operations of F_1 (order of F_1), the number of left cosets in the decomposition (3.4.2.10) is

$$n = [G : F_1] = |G| : |F_1|, \quad (3.4.2.11)$$

where $|G|$, $|F_1|$ are orders of the point groups G , F_1 , respectively. The index n is a quantitative measure of the degree of dissymmetrization $G \supset F_1$. Thus the number of principal domain states in orbit $G\mathbf{S}_1$ is equal to the index of F_1 in G , i.e. to the number of operations of the high-symmetry group G divided by the number of operations of the low-symmetry phase F_1 . In our illustrative example we get $n = |4_z/m_z m_x m_{xy}| : |2_x m_y m_z| = 16 : 4 = 4$.

The basic formula (3.4.2.11) expresses a remarkable result: the number n of principal domain states is determined by how many times the number of symmetry operations increases at the transition from the low-symmetry group F_1 to the high-symmetry group G , or, the other way around, the fraction $\frac{1}{n}$ is a quantitative measure of the symmetry decrease from G to F_1 , $|F_1| = \frac{1}{n} |G|$. Thus it is not the concrete structural change, nor even the particular symmetries of both phases, but only the extent of dissymmetrization that determines the number of principal domain states. This conclusion illustrates the fundamental role of symmetry in domain structures.

(2) Relation (3.4.2.9) yields a recipe for calculating all principal domain states of the orbit $G\mathbf{S}_1$: One applies successively to the first principal domain states \mathbf{S}_1 the representatives of all left cosets of F_1 :

$$G\mathbf{S}_1 = \{\mathbf{S}_1, g_2 \mathbf{S}_1, \dots, g_j \mathbf{S}_1, \dots, g_n \mathbf{S}_1\}, \quad (3.4.2.12)$$

where the operations $g_1 = e, g_2, \dots, g_j, \dots, g_n$ are the representatives of left cosets in the decomposition (3.4.2.10) and e is an identity operation. We add that any operation of a left coset can be chosen as its representative, hence the operation g_j can be chosen arbitrarily from the left coset $g_j F_1, j = 1, 2, \dots, n$.

This result can be illustrated in our example. Table 3.4.2.1 presents in the first column the four left cosets $g_j \{2_x m_y m_z\}$ of the group $F_1 = 2_x m_y m_z$. The corresponding principal domain states $\mathbf{S}_j, j = 1, 2, 3, 4$, and the values of spontaneous polarization in these principal domain states are given in the second and the third columns, respectively. It is easy to verify in Fig. 3.4.2.2 that all operations of each left coset transform the first principal domain state \mathbf{S}_1 into one principal domain state $\mathbf{S}_j, j = 2, 3, 4$.

The left coset decompositions of all crystallographic point groups and their subgroup symmetry are available in the software *GI★KoBo-1*, path: *Subgroups\View\Twinning Group*.

Table 3.4.2.1. Left and double cosets, principal and secondary domain states and their tensor parameters for the phase transition with $G = 4_z/m_z m_x m_{xy}$ and $F_1 = 2_x m_y m_z$

($\pm P00$) and ($0\pm P0$): polarization; ($000\pm g00$) and ($0000\pm g0$): optical activity; u_1, u_2 : strain; s_{11}, s_{22} : elastic compliances (see Fig. 3.4.3.5).

Left cosets $g_j \mathbf{S}_1$				Principal domain states			Secondary domain states		
1	2_x	m_y	m_z	\mathbf{S}_1	(P00)	(000g00)	\mathbf{R}_1	$u_1 - u_2$	$s_{11} - s_{22}$
$\bar{1}$	m_x	2_y	2_z	\mathbf{S}_2	(-P00)	(000-g00)			
2_{xy}	4_z	$\bar{4}_z^3$	m_{xy}	\mathbf{S}_3	(0P0)	(0000-g0)	\mathbf{R}_2	$u_2 - u_1$	$s_{22} - s_{11}$
$2_{x\bar{y}}$	4_z^3	$\bar{4}_z$	m_{xy}	\mathbf{S}_4	(0-P0)	(0000g0)			