

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

Let us turn briefly to the symmetries of the principal domain states. From Fig. 3.4.2.2 we deduce that two domain states \mathbf{S}_1 and \mathbf{S}_2 in our illustrative example have the same symmetry, $F_1 = F_2 = 2_x m_y m_z$, whereas two others \mathbf{S}_3 and \mathbf{S}_4 have another symmetry, $F_3 = F_4 = m_x 2_y m_z$. We see that symmetry does not specify the principal domain state in a unique way, although a principal domain state \mathbf{S}_j has a unique symmetry $F_i = I_G(\mathbf{S}_j)$.

It turns out that if g_j transforms \mathbf{S}_1 into \mathbf{S}_j , then the symmetry group F_j of \mathbf{S}_j is conjugate by g_j to the symmetry group F_1 of \mathbf{S}_1 [see Section 3.2.3.3, Proposition 3.2.3.13 and equation (3.2.3.55)]:

$$\text{if } \mathbf{S}_j = g_j \mathbf{S}_1, \text{ then } F_j = g_j F_1 g_j^{-1}. \quad (3.4.2.13)$$

One can easily check that in our example each operation of the second left coset of $F_1 = 2_x m_y m_z$ (second row in Table 3.4.2.1) transforms $F_1 = 2_x m_y m_z$ into itself, whereas operations from the third and fourth left cosets yield $F_3 = F_4 = m_x 2_y m_z$. We shall return to this issue again at the end of Section 3.4.2.2.3.

3.4.2.2. Degenerate (secondary) domain states, partition of principal domain states

In this section we demonstrate that any morphic (spontaneous) property appears in the low-symmetry phase in several equivalent variants and find what determines their number and basic properties.

As we saw in Fig. 3.4.2.2, the spontaneous polarization – a principal tensor parameter of the $4_z/m_z m_x m_{xy} \supset 2_x m_y m_z$ phase transition – can appear in four different directions that define four principal domain states. Another morphic property is a spontaneous strain describing the change of unit-cell shape; it is depicted in Fig. 3.4.2.2 as a transformation of a square into a rectangle. This change can be expressed by a difference between two strain components $u_{11} - u_{22} = \lambda^{(1)}$, which is a morphic tensor parameter since it is zero in the parent phase and nonzero in the ferroic phase. The quantity $\lambda^{(1)} = u_{11} - u_{22}$ is a secondary order parameter of the transition $4_z/m_z m_x m_{xy} \supset 2_x m_y m_z$ (for secondary order parameters see Section 3.1.3.2).

From Fig. 3.4.2.2, we see that two domain states \mathbf{S}_1 and \mathbf{S}_2 have the same spontaneous strain, whereas \mathbf{S}_3 and \mathbf{S}_4 exhibit another spontaneous strain $\lambda^{(2)} = u_{22} - u_{11} = -\lambda^{(1)}$. Thus we can infer that a property ‘to have the same value of spontaneous strain’ divides the four principal domain states $\mathbf{S}_1, \mathbf{S}_2, \mathbf{S}_3$ and \mathbf{S}_4 into two classes: \mathbf{S}_1 and \mathbf{S}_2 with the same spontaneous strain $\lambda^{(1)}$ and \mathbf{S}_3 and \mathbf{S}_4 with the same spontaneous strain $\lambda^{(2)} = -\lambda^{(1)}$. Spontaneous strain appears in two ‘variants’: $\lambda^{(1)}$ and $\lambda^{(2)} = -\lambda^{(1)}$.

We can define a *ferroelastic domain state* as a state of the crystal with a certain value of spontaneous strain λ , irrespective of the value of the principal order parameter. Values $\lambda = \lambda^{(1)}$ and $\lambda^{(2)} = -\lambda^{(1)}$ thus specify two ferroelastic domain states \mathbf{R}_1 and \mathbf{R}_2 , respectively. The spontaneous strain in this example is a secondary order parameter and the ferroelastic domain states can therefore be called *degenerate (secondary) domain states*.

An algebraic version of the above consideration can be deduced from Table 3.4.2.1, where to each principal domain state (given in the second column) there corresponds a left coset of $F_1 = 2_x m_y m_z$ (presented in the first column). Thus to the partition of principal domain states into two subsets

$$\{\mathbf{S}_1, \mathbf{S}_2, \mathbf{S}_3, \mathbf{S}_4\} = \{\mathbf{S}_1, \mathbf{S}_2\}_{\lambda^{(1)}} \cup \{\mathbf{S}_3, \mathbf{S}_4\}_{\lambda^{(2)}}, \quad (3.4.2.14)$$

there corresponds, according to relation (3.4.2.9), a partition of left cosets

$$\begin{aligned} 4_z/m_z m_x m_{xy} \\ &= \{2_x m_y m_z\} \cup \bar{1}\{2_x m_y m_z\} \cup \{2_{xy}\{2_x m_y m_z\} \cup 2_{xy}\{2_x m_y m_z\}\} \\ &= m_x m_y m_z \cup 2_{xy}\{m_x m_y m_z\}, \end{aligned} \quad (3.4.2.15)$$

where we use the fact that the union of the first two left cosets of $2_x m_y m_z$ is equal to the group $m_x m_y m_z$. This group is the stabilizer

of the first ferroelastic domain state \mathbf{R}_1 , $I_G(\mathbf{R}_1) = m_x m_y m_z$. Two left cosets of $m_x m_y m_z$ correspond to two ferroelastic domain states, \mathbf{R}_1 and \mathbf{R}_2 , respectively. Therefore, the number n_a of ferroelastic domain states is equal to the number of left cosets of $m_x m_y m_z$ in $4_z/m_z m_x m_{xy}$, i.e. to the index of $m_x m_y m_z$ in $4_z/m_z m_x m_{xy}$, $n_a = [4_z/m_z m_x m_{xy} : m_x m_y m_z] = |4_z/m_z m_x m_{xy}| : |m_x m_y m_z| = 16 : 8 = 2$, and the number d_a of principal domain states in one ferroelastic domain state is equal to the index of $2_x m_y m_z$ in $m_x m_y m_z$, i.e. $d_a = [m_x m_y m_z : 2_x m_y m_z] = |m_x m_y m_z| : |2_x m_y m_z| = 8 : 4 = 2$.

A generalization of these considerations, performed in Section 3.2.3.3.5 (see especially Proposition 3.2.3.30 and Examples 3.2.3.10 and 3.2.3.33), yields the following main results.

Assume that $\lambda^{(1)}$ is a secondary order parameter of a transition with symmetry descent $G \supset F_1$. Then the stabilizer L_1 of this parameter $I_G(\lambda^{(1)}) \equiv L_1$ is an intermediate group,

$$F_1 \subseteq I_G(\lambda^{(1)}) \equiv L_1 \subseteq G. \quad (3.4.2.16)$$

Lattices of subgroups in Figs. 3.1.3.1 and 3.1.3.2 are helpful in checking this condition.

The set of n principal domain states (the orbit $G\mathbf{S}_1$) splits into n_λ subsets

$$n_\lambda = [G : L_1] = |G| : |L_1|. \quad (3.4.2.17)$$

Each of these subsets consists of d_λ principal domain states,

$$d_\lambda = [L_1 : F_1] = |L_1| : |F_1|. \quad (3.4.2.18)$$

The number d_λ is called a *degeneracy of secondary domain states*.

The product of numbers n_λ and d_λ is equal to the number n of principal domain states [see equation (3.2.3.26)]:

$$n_\lambda d_\lambda = n. \quad (3.4.2.19)$$

Principal domain states from each subset have the same value of the secondary order parameter $\lambda^{(j)}$, $j = 1, 2, \dots, n_\lambda$, and any two principal domain states from different subsets have different values of $\lambda^{(j)}$. A state of the crystal with a given value of the secondary order parameter $\lambda^{(j)}$ will be called a *secondary domain state* \mathbf{R}_j , $j = 1, 2, \dots, n_\lambda$. Equivalent terms are *degenerate* or *compound domain state*.

In a limiting case $L_1 = F_1$, the parameter $\lambda^{(1)}$ is identical with the principal tensor parameter and there is no degeneracy, $d_\lambda = 1$.

Secondary domain states $\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_j, \dots, \mathbf{R}_{n_\lambda}$ are in a one-to-one correspondence with left cosets of L_1 in the decomposition

$$G = h_1 L_1 \cup h_2 L_1 \cup \dots \cup h_j L_1 \cup \dots \cup h_{n_\lambda} L_1, \quad (3.4.2.20)$$

therefore

$$\mathbf{R}_j = h_j \mathbf{R}_1, \quad j = 1, 2, \dots, n_\lambda. \quad (3.4.2.21)$$

Principal domain states of the first secondary domain state \mathbf{R}_1 can be determined from the first principal domain state \mathbf{S}_1 :

$$\mathbf{S}_k = p_k \mathbf{S}_1, \quad k = 1, 2, \dots, d_\lambda, \quad (3.4.2.22)$$

where p_k is the representative of the k th left coset of F_1 of the decomposition

$$L_1 = p_1 F_1 \cup p_2 F_1 \cup \dots \cup p_k F_1 \cup \dots \cup p_{d_\lambda} F_1. \quad (3.4.2.23)$$

The partition of principal domain states according to a secondary order parameter offers a convenient labelling of principal domain states by two indices j, k , where the first index j denotes the sequential number of the secondary domain state and the second index k gives the sequential number of the principal domain state within the j th secondary domain state [see equation (3.2.3.79)]:

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$$\mathbf{S}_{jk} = h_j p_k \mathbf{S}_{11}, \quad \mathbf{S}_{11} = \mathbf{S}_1, \quad j = 1, 2, \dots, n_\lambda, \quad k = 1, 2, \dots, d_\lambda, \quad (3.4.2.24)$$

where h_j and p_k are representatives of the decompositions (3.4.2.20) and (3.4.2.23), respectively.

The secondary order parameter λ can be identified with a principal order parameter of a phase transition with symmetry descent $G \subset L_1$ (see Section 3.4.2.3). The concept of secondary domain states enables one to define domain states that are characterized by a certain spontaneous property. We present the three most significant cases of such ferroic domain states.

3.4.2.2.1. Ferroelastic domain state

The distinction ferroelastic–non-ferroelastic is a basic division in domain structures. *Ferroelastic transitions* are ferroic transitions involving a spontaneous distortion of the crystal lattice that entails a change of shape of the crystallographic or conventional unit cell (Wadhawan, 2000). Such a transformation is accompanied by a change in the number of independent nonzero components of a symmetric second-rank tensor u that describes spontaneous strain.

In discussing ferroelastic and non-ferroelastic domain structures, the concepts of crystal family and holohedry of a point group are useful (IT A, 2005). Crystallographic point groups (and space groups as well) can be divided into seven crystal systems and six *crystal families* (see Table 3.4.2.2). A symmetry descent within a crystal family does not entail a qualitative change of the spontaneous strain – the number of independent nonzero tensor components of the strain tensor u remains unchanged.

We shall call the largest group of the crystal family to which the group M belongs the *family group of M* (symbol $\text{Fam}M$). Then a simple criterion for a ferroic phase transition with symmetry descent $G \subset F$ to be a *non-ferroelastic phase transition* is

$$F \subset G, \quad \text{Fam}F = \text{Fam}G. \quad (3.4.2.25)$$

A necessary and sufficient condition for a *ferroelastic phase transition* is

$$F \subset G, \quad \text{Fam}F \neq \text{Fam}G. \quad (3.4.2.26)$$

A *ferroelastic domain state* \mathbf{R}_i is defined as a state with a homogeneous spontaneous strain $u^{(i)}$. [We drop the suffix ‘s’ or ‘(s)’ if the serial number of the domain state is given as the superscript (i). The definition of spontaneous strain is given in Section 3.4.3.6.1.] Different ferroelastic domain states differ in spontaneous strain. The symmetry of a ferroelastic domain state \mathbf{R}_i is specified by the stabilizer $I_G(u^{(i)})$ of the spontaneous strain $u^{(i)}$ of the principal domain state \mathbf{S}_i [see (3.4.2.16)]. This stabilizer, which we shall denote by A_i , can be expressed as an intersection of the parent group G and the family group of F_i (see Table 3.4.2.2):

$$A_i \equiv I_G(u^{(i)}) = G \cap \text{Fam}F_i. \quad (3.4.2.27)$$

This equation indicates that the ferroelastic domain state \mathbf{R}_i has a prominent single-domain orientation. Further on, the term ‘ferroelastic domain state’ will mean a ‘ferroelastic domain state in single-domain orientation’.

In our illustrative example,

$$\begin{aligned} A_1 &= I_{4_z/m_z m_x m_{xy}}(u_{11} - u_{22}) \\ &= \text{Fam}(2_x m_y m_z) \cap m 4_z / m_z m_x m_{xy} \\ &= m_x m_y m_z \cap 4_z / m_z m_x m_{xy} = m_x m_y m_z. \end{aligned}$$

The number n_a of ferroelastic domain states is given by

$$n_a = [G : A_1] = |G| : |A_1|. \quad (3.4.2.28)$$

In our example, $n_a = |4_z/m_z m_x m_{xy}| : |m_x m_y m_z| = 16 : 8 = 2$. In Table 3.4.2.7, last column, the number n_a of ferroelastic domain states is given for all possible ferroic phase transitions.

The number d_a of principal domain states compatible with one ferroelastic domain state (degeneracy of ferroelastic domain states) is given by

$$d_a = [A_1 : F_1] = |A_1| : |F_1|. \quad (3.4.2.29)$$

In our example, $d_a = |m_x m_y m_z| : |2_x m_y m_z| = 8 : 4 = 2$, i.e. two non-ferroelastic principal domain states are compatible with each of the two ferroelastic domain states (cf. Fig. 3.4.2.2).

The product of n_a and d_a is equal to the number n of all principal domain states [see equation (3.4.2.19)],

$$n_a d_a = [G : A_1][A_1 : F_1] = [G : F_1] = n. \quad (3.4.2.30)$$

The number d_a of principal domain states in one ferroelastic domain state can be calculated for all ferroic phase transitions from the ratio of numbers n and n_a that are given in Table 3.4.2.7.

According to Aizu (1969), we can recognize three possible cases (see also Table 3.4.2.3):

(i) *Full ferroelastics*: All principal domain states differ in spontaneous strain. In this case, $n_a = n$, i.e. $A_1 = F_1$, ferroelastic domain states are identical with principal domain states.

(ii) *Partial ferroelastics*: Some but not all principal domain states differ in spontaneous strain. A necessary and sufficient condition is $1 < n_a < n$, or, equivalently, $F_1 \subset A_1 \subset G$. In this case, ferroelastic domain states are degenerate secondary domain states with degeneracy $n > d_a = |A_1| : |F_1| > 1$. In this case, the phase transition $G \supset F_1$ can also be classified as an *improper ferroelastic* one (see Section 3.1.3.2).

(iii) *Non-ferroelastics*: All principal domain states have the same spontaneous strain. The criterion is $n_a = 1$, i.e. $A_1 = G$.

Example 3.4.2.1. Domain states in leucite. Leucite (KAlSi_2O_6) (see e.g. Hatch *et al.*, 1990) undergoes at about 938 K a ferroelastic phase transition from cubic symmetry $G = m\bar{3}m$ to tetragonal symmetry $L = 4/mmm$. This phase can appear in $|m\bar{3}m| : |4/mmm| = 3$ single-domain states, which we denote \mathbf{R}_1 , \mathbf{R}_2 , \mathbf{R}_3 . The symmetry group of the first domain state \mathbf{R}_1 is

Table 3.4.2.2. Crystal systems, holohedries, crystal families and number of spontaneous strain components

Point group M	Crystal system	Holohedry Hol M	Spontaneous strain components		Crystal family	Family group Fam M
			Independent	Nonzero		
23, $m\bar{3}$, 432, $\bar{4}3m$, $m\bar{3}m$	Cubic	$m\bar{3}m$	1	3	Cubic	$m\bar{3}m$
6, $\bar{6}$, $6/m$, 622, $6mm$, $\bar{6}2m$, $6/mmm$	Hexagonal	$6/mmm$	2	3	Hexagonal	$6/mmm$
3, $\bar{3}$, 32, $3m$, $\bar{3}m$	Trigonal	$\bar{3}m$	2	3		
4, $\bar{4}$, $4/m$, 422, $4mm$, $\bar{4}2m$, $4/mmm$	Tetragonal	$4/mmm$	2	3	Tetragonal	$4/mmm$
222, $mm2$, mmm	Orthorhombic	mmm	3	3	Orthorhombic	mmm
2, m , $2/m$	Monoclinic	$2/m$	4	4	Monoclinic	$2/m$
1, $\bar{1}$	Triclinic	$\bar{1}$	6	6	Triclinic	$\bar{1}$

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Table 3.4.2.3. Classification of ferroic phases according to ferroelastic and ferroelectric domain states

n_e , n_a and n : number of ferroelectric, ferroelastic and principal domain states, respectively. Terms in parentheses were introduced by Aizu (1970a).

Ferroelastic			Ferroelectric			
$n_a = n$	$1 < n_a < n$	$n_a = 1$	$n_e = n$	$1 < n_e < n$	$n_e = 1$	$n_e = 0$
faithful (full)	degenerate (partial)	non-ferroelastic (non-ferroelastic)	faithful (full)	degenerate (partial)	trivial	zero
f or af	d or ad	n or an	f or ef	d or ed	t or et	z or ez
					non-ferroelectric (non-ferroelectric)	
					n or en	

$L_1 = 4_x/m_x m_y m_z$. This group equals the stabilizer $I_G(u^{(1)})$ of the spontaneous strain $u^{(1)}$ of \mathbf{R}_1 since $\text{Fam}(4_x/m_x m_y m_z) = 4_x/m_x m_y m_z$ (see Table 3.4.2.2), hence this phase is a full ferroelastic one.

At about 903 K, another phase transition reduces the symmetry $4/mmm$ to $F = 4/m$. Let us suppose that this transition has taken place in a domain state \mathbf{R}_1 with symmetry $L_1 = 4_x/m_x m_y m_z$; then the room-temperature ferroic phase has symmetry $F_1 = 4_x/m_x$. The $4_x/m_x m_y m_z \supset 4_x/m_x$ phase transition is a non-ferroelastic one [$\text{Fam}(4_x/m_x) = 4_x/m_x m_y m_z$] with $|4_x/m_x m_y m_z| : |4_x/m_x| = 8 : 4 = 2$ non-ferroelastic domain states, which we denote \mathbf{S}_1 and \mathbf{S}_2 . Similar considerations performed with initial domain states \mathbf{R}_2 and \mathbf{R}_3 generate another two couples of principal domain states $\mathbf{S}_3, \mathbf{S}_4$ and $\mathbf{S}_5, \mathbf{S}_6$, respectively. Thus the room-temperature phase is a partially ferroelastic phase with three degenerate ferroelastic domain states, each of which can contain two principal domain states. Both ferroelastic domains and non-ferroelastic domains within each ferroelastic domain have been observed [see Fig. 3.3.10.13 in Chapter 3.3, Palmer *et al.* (1988) and Putnis (1992)].

3.4.2.2.2. Ferroelectric domain states

Ferroelectric domain states are defined as states with a homogeneous spontaneous polarization; different ferroelectric domain states differ in the direction of the spontaneous polarization. Ferroelectric domain states are specified by the stabilizer $I_G(\mathbf{P}_s^{(1)})$ of the spontaneous polarization $\mathbf{P}_s^{(1)}$ in the first principal domain state \mathbf{S}_1 [see equation (3.4.2.16)]:

$$F_1 \subseteq C_1 \equiv I_G(\mathbf{P}_s^{(1)}) \subseteq G. \quad (3.4.2.31)$$

The stabilizer C_1 is one of ten polar groups: 1, 2, 3, 4, 6, m , $mm2$, $3m$, $4mm$, $6mm$. Since F_1 must be a polar group too, it is simple to find the stabilizer C_1 fulfilling relation (3.4.2.31).

The number n_e of ferroelectric domain states is given by

$$n_e = [G : C_1] = |G| : |C_1|. \quad (3.4.2.32)$$

If the polar group C_1 does not exist, we put $n_e = 0$. The number n_e of ferroelectric domain states is given for all ferroic phase transitions in the eighth column of Table 3.4.2.7.

The number d_a of principal domain states compatible with one ferroelectric domain state (degeneracy of ferroelectric domain states) is given by

$$d_e = [C_1 : F_1] = |C_1| : |F_1|. \quad (3.4.2.33)$$

The product of n_e and d_e is equal to the number n of all principal domain states [see equation (3.4.2.19)],

$$n_e d_e = n. \quad (3.4.2.34)$$

The degeneracy d_e of ferroelectric domain states can be calculated for all ferroic phase transitions from the ratio of the numbers n and n_e that are given in Table 3.4.2.7.

Aizu (1969, 1970a) recognizes three possible cases (see also Table 3.4.2.3):

(i) *Full ferroelectrics*: All principal domain states differ in spontaneous polarization. In this case, $n_e = n$, *i.e.* $C_1 = F_1$, ferroelectric domain states are identical with principal domain states.

(ii) *Partial ferroelectrics*: Some but not all principal domain states differ in spontaneous polarization. A necessary and sufficient condition is $1 < n_e < n$, or equivalently, $F_1 \subset C_1 \subset G$. Ferroelectric domain states are degenerate secondary domain states with degeneracy $n > d_e > 1$. In this case, the phase transition $G \supset F_1$ can be classified as an *improper ferroelectric* one (see Section 3.1.3.2).

(iii) *Non-ferroelectrics*: No principal domain states differ in spontaneous polarization. There are two possible cases: (a) The parent phase is polar; then $C_1 = G$ and $n_e = 1$. (b) The parent phase is non-polar; in this case a polar stabilizer C_1 does not exist, then we put $n_e = 0$.

The classification of full-, partial- and non-ferroelectrics and ferroelastics is summarized in Table 3.4.2.3.

Results for all symmetry descents follow readily from the numbers n , n_a , n_e in Table 3.4.2.7 and are given for all symmetry descents in Aizu (1970a). One can conclude that partial ferroelectrics are rather rare.

Example 3.4.2.3. Domain structure in tetragonal perovskites. Some perovskites (*e.g.* barium titanate, BaTiO_3) undergo a phase transition from the cubic parent phase with $G = m\bar{3}m$ to a tetragonal ferroelectric phase with symmetry $F_1 = 4_x m_y m_z$. The stabilizer $A_1 = \text{Fam}(4_x m_y m_z) \cap m\bar{3}m = 4_x/m_x m_y m_z$. There are $n_a = |m\bar{3}m| : |4_x/m_x m_y m_z| = 3$ ferroelastic domain states each compatible with $d_a = |4_x/m_x m_y m_z| : |4_x m_y m_z| = 2$ principal ferroelectric domain states that are related *e.g.* by inversion $\bar{1}$, *i.e.* spontaneous polarization is antiparallel in two principal domain states within one ferroelastic domain state.

A similar situation, *i.e.* two non-ferroelastic domain states with antiparallel spontaneous polarization compatible with one ferroelastic domain state, occurs in perovskites in the trigonal ferroic phase with symmetry $F = 3m$ and in the orthorhombic ferroic phase with symmetry $F_1 = m_{xy} 2_{xy} m_z$.

Many other examples are discussed by Newnham (1974, 1975), Newnham & Cross (1974a,b), and Newnham & Skinner (1976).

3.4.2.2.3. Domain states with the same stabilizer

In our illustrative example (see Fig. 3.4.2.2), we have seen that two domain states \mathbf{S}_1 and \mathbf{S}_2 have the same symmetry group (stabilizer) $2_x m_y m_z$. In general, the condition 'to have the same stabilizer (symmetry group)' divides the set of n principal domain states into equivalence classes. As shown in Section 3.2.3.3, the role of an intermediate group L_1 is played in this case by the normalizer $N_G(F_1)$ of the symmetry group F_1 of the first domain state \mathbf{S}_1 . The number d_F of domain states with the same symmetry group is given by [see Example 3.2.3.34 in Section 3.2.3.3.5 and equation (3.2.3.95)],

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$$d_F = [N_G(F_1) : F_1] = |N_G(F_1)| : |F_1|. \quad (3.4.2.35)$$

The number n_F of subgroups that are conjugate under G to F_1 can be calculated from the formula [see equation (3.2.3.96)]

$$n_F = [G : N_G(F_1)] = |G| : |N_G(F_1)|. \quad (3.4.2.36)$$

The product of n_F and d_F is equal to the number n of ferroic domain states,

$$n = n_F d_F. \quad (3.4.2.37)$$

The normalizer $N_G(F_1)$ enables one not only to determine which domain states have the symmetry F_1 but also to calculate all subgroups that are conjugate under G to F_1 (see Examples 3.2.3.22, 3.2.3.29 and 3.2.3.34 in Section 3.2.3.3).

Normalizers $N_G(F_1)$ and the number d_F of principal domain states with the same symmetry are given in Table 3.4.2.7 for all symmetry descents $G \supset F_1$. The number n_F of subgroups conjugate to F_1 is given by $n_F = n : d_F$.

All these results obtained for point-group symmetry descents can be easily generalized to microscopic domain states and space-group symmetry descents (see Section 3.4.2.5).

3.4.2.3. Property tensors associated with ferroic domain states

In the preceding section we derived relations for domain states without considering their specific physical properties. Basic formulae for the number of principal and secondary domain states [see equations (3.4.2.11) and (3.4.2.17), respectively] and the transformation properties of these domain states [equations (3.4.2.12) and (3.4.2.21), respectively] follow immediately from the symmetry groups G , F_1 of the parent and ferroic phases, respectively. Now we shall examine which components of property tensors specify principal and secondary domain states and how these tensor components change in different domain states.

A property tensor τ is specified by its components. The number $m_i(\tau)$ of independent tensor components of a certain tensor τ depends on the point-group symmetry G of the crystal (see Chapter 1.1). The number $m_c(\tau)$ of nonzero Cartesian (rectangular) components depends on the orientation of the crystal in the reference Cartesian coordinate system and is equal to, or greater than, the number $m_i(\tau)$ of independent tensor components; this number $m_i(\tau)$ is independent of orientation. Then there are $m_c(\tau) - m_i(\tau)$ linear relations between Cartesian tensor components. The difference $m_c(\tau) - m_i(\tau)$ is minimal for a 'standard' orientation, in which symmetry axes of the crystal are, if possible, parallel to the axes of the reference coordinate system [for more on this choice, see Nye (1985) Appendix B, Sirotnin & Shaskolskaya (1982), Shuvalov (1988) and *IEEE Standards on Piezoelectricity* (1987)]. Even in this standard orientation, only for point groups of triclinic, monoclinic and orthorhombic crystal systems is the number $m_c(\tau)$ of nonzero Cartesian components of each property tensor equal to the number $m_i(\tau)$ of independent tensor components, *i.e.* all Cartesian tensor components are independent. For all other point groups $m_c(\tau) - m_i(\tau) > 0$, *i.e.* there are always relations between some Cartesian tensor components. One can verify this statement for the strain tensor in Table 3.4.2.2.

The relations between Cartesian tensor components can be removed when one uses *covariant tensor components*. [Kopský (1979); see also the manual of the the software *GI★KoBo-1* and Kopský (2001). An analogous decomposition of Cartesian tensors into irreducible parts has been performed by Jerphagnon *et al.* (1978).] Covariant tensor components are linear combinations of Cartesian tensor components that transform according to irreducible matrix representations $D^{(\omega)}(G)$ of the group G of the crystal (*i.e.* they form a basis of irreducible representations of G ; see Chapter 1.2). The number of covariant tensor

components equals the number of independent components of the tensor τ .

The advantage of expressing property tensors by covariant tensor components becomes obvious when one considers a change of a property tensor at a ferroic phase transition. A symmetry descent $G \supset F_1$ is accompanied by the preservation of, or an increase of, the number of independent Cartesian tensor components. The latter possibility can manifest itself either by the appearance of morphic Cartesian tensor components in the low-symmetry phase or by such changes of nonzero Cartesian components that break some relations between tensor components in the high-symmetry phase. This is seen in our illustrative example of the strain tensor u . In the high-symmetry phase with $G = 4_2/m_z m_x m_{xy}$, the strain tensor has two independent components and three nonzero components: $u_{11} \neq u_{22} = u_{33}$. In the low-symmetry phase with $F_1 = 2_x m_y m_z$, there are three independent and three nonzero components: $u_{11} \neq u_{22} \neq u_{33}$, *i.e.* the equation $u_{22} = u_{33}$ does not hold in the parent phase. This change cannot be expressed by a single Cartesian morphic component.

Since there are no relations between covariant tensor components, any change of tensor components at a symmetry descent can be expressed by morphic covariant tensor components, which are zero in the parent phase and nonzero in the ferroic phase. In our example, the covariant tensor component of the spontaneous strain is $u_{11} - u_{22}$, which is a morphic component since $u_{11} - u_{22} = 0$ for the symmetry $4_2/m_z m_x m_{xy}$ but $u_{11} - u_{22} \neq 0$ for symmetry $2_x m_y m_z$.

Tensorial covariants are defined in an exact way in the manual of the software *GI★KoBo-1* and in Kopský (2001). Here we give only a brief account of this notion. Consider a crystal with symmetry G and a property tensor τ with n_τ independent tensor components. Let $D^{(\omega)}(G)$ be a d_α -dimensional physically irreducible matrix representation of G . The $D^{(\omega)}(G)$ *covariant* of τ consists of the following d_α *covariant tensor components*: $\tau_a^\alpha = (\tau_{a,1}^\alpha, \tau_{a,2}^\alpha, \dots, \tau_{a,d_\alpha}^\alpha)$, where $a = 1, 2, \dots$ and $m = n_\tau/d_\alpha$ numbers different d_α -tuples formed from n_τ components of τ . These covariant tensor components are linear combinations of Cartesian components of τ that transform as so-called typical variables of the matrix representation $D^{(\omega)}(G)$, *i.e.* the transformation properties under operations $g \in G$ of covariant tensor components are expressed by matrices $D^{(\omega)}(g)$.

The relation between two presentations of the tensor τ is provided by *conversion equations*, which express Cartesian tensor components as linear combinations of covariant tensor components and *vice versa* [for details see the manual and Appendix E of the software *GI★KoBo-1* and Kopský (2001)].

Tensorial covariants for all non-equivalent physically irreducible matrix representations of crystallographic point groups and all important property tensors up to rank four are listed in the software *GI★KoBo-1* and in Kopský (2001). Thus, for example, in Table D of the software *GI★KoBo-1*, or in Kopský (2001) p. 5, one finds for the two-dimensional irreducible representation E of group 422 the following tensorial covariants: (P_1, P_2) , (d_{11}, d_{22}) , (d_{12}, d_{21}) , (d_{13}, d_{23}) , (d_{26}, d_{16}) , (d_{35}, d_{34}) .

Let us denote by $\tau_a^{(\omega(1))}$ a tensorial covariant of τ in the first single-domain state \mathbf{S}_1 . A crucial role in the analysis is played by the stabilizer $I_G(\tau_a^{(\omega(1))})$ of these covariants, *i.e.* all operations of the parent group G that leave $\tau_a^{(\omega(1))}$ invariant. There are three possible cases:

(1) If

$$I_G(\tau_a^{(\omega(1))}) = G, \quad (3.4.2.38)$$

then all components of $\tau_a^{(\omega(1))}$ that are nonzero in the parent phase are also nonzero in the ferroic phase. All these components are the same in all principal domain states. For important property tensors and for all point groups G , these covariant tensor components are listed in the main tables of the software