

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

explained in Section 3.2.3, but the important points are illustrated with simple examples comprehensible even without mathematical details. The synoptic tables in Sections 3.4.2 and 3.4.3 present the main results of the analysis for all possible ferroic domain structures. More detailed information on certain points can be found in the software *GI★KoBo-1*.

All these results are definite – their validity does not depend on any particular model or approximation – and form thus a firm basis for further more detailed quantitative treatments. ‘*For the most part, the only exact statements which can be made about a solid state system are those which arise as a direct consequence of symmetry alone.*’ (Knox & Gold, 1967.)

The exposition starts with domain states, continues with pairs of domain states and domain distinction, and terminates with domain twins and walls. This is also the sequence of steps in domain-structure analysis, which proceeds from the simplest to more complicated objects.

In Section 3.4.2, we explain the concept of *domain states* (also called variants or orientational states), define different types of domain states (principal, ferroelastic, ferroelectric, basic), find simple formulae for their number, and disclose their hierarchy and relation with symmetry lowering and with order parameters of the transition. Particular results for all possible ferroic phase transitions can be found in synoptic Table 3.4.2.7, which lists all possible crystallographically non-equivalent *point-group symmetry descents that may appear at a ferroic phase transition*. For each descent, all independent twinning groups (characterizing the relation between two domain states) are given together with the number of principal, ferroelastic and ferroelectric domain states and other data needed in further analysis.

Section 3.4.3 deals with *pairs of domain states* and with the relationship between two domain states in a pair. This relationship, in mineralogy called a ‘twin law’, determines the distinction between domain states, specifies switching processes between two domain states and forms a starting point for discussing domain walls and twins. We show different ways of expressing the relation between two domain states of a domain pair, derive a classification of domain pairs, find non-equivalent domain pairs and determine which tensor properties are different and which are the same in two domain states of a domain pair.

The presentation of non-equivalent domain pairs is divided into two parts. Synoptic Table 3.4.3.4 lists all representative *non-equivalent non-ferroelastic domain pairs*, and for each pair gives the twinning groups, and the number of tensor components that are different and that are the same in two domain states. These numbers are given for all important property tensors up to rank four. We also show how these data can be used to determine switching forces between two non-ferroelastic domain states.

Then we explain specific features of ferroelastic domain pairs: compatible (permissible) domain walls and disorientation of domain states in ferroelastic domain twins. A list of all non-equivalent ferroelastic domain pairs is presented in two tables. Synoptic Table 3.4.3.6 contains all *non-equivalent ferroelastic domain pairs with compatible (coherent) domain walls*. This table gives the orientation of compatible walls and their symmetry properties. Table 3.4.3.7 lists all *non-equivalent ferroelastic domain pairs with no compatible ferroelastic domain walls*.

Column K_{1j} in Table 3.4.2.7 specifies all representative non-equivalent domain pairs that can appear in each particular phase transition; in combination with Tables 3.4.3.4 and 3.4.3.6, it allows one to determine the main features of any ferroic domain structure.

Section 3.4.4 is devoted to domain twins and domain walls. We demonstrate that the symmetry of domain twins and domain walls is described by layer groups, give a classification of domain twins and walls based on their symmetry, and present possible layer groups of non-ferroelastic and ferroelastic domain twins and walls. Then we discuss the properties of finite-thickness domain walls. In an example, we illustrate the symmetry analysis

of microscopic domain walls and present conclusions that can be drawn from this analysis about the microscopic structure of domain walls.

The exposition is given in the continuum description with crystallographic point groups and property tensors. In this approach, all possible cases are often treatable and where possible are covered in synoptic tables or – in a more detailed form – in the software *GI★KoBo-1*. Although the group-theoretical tools are almost readily transferable to the microscopic description (using the space groups and atomic positions), the treatment of an inexhaustible variety of microscopic situations can only be illustrated by particular examples.

Our attempt to work with well defined notions calls for introducing several new, and generalizing some accepted, concepts. Also an extended notation for the symmetry operations and groups has turned out to be indispensable. Since there is no generally accepted terminology on domain structures yet, we often have to choose a term from several existing more-or-less equivalent variants.

The specialized scope of this chapter does not cover many other important aspects of domain-structure studies. More information can be found in the following references. The only comprehensive monograph, by Tagancev *et al.* (2010), provides a thorough treatise on major topics of domain structure in non-magnetic ferroic crystals and thin films. There are two specialized monographs: the booklet by Fesenko *et al.* (1990) deals with experimental aspects of domain structure in multi-axial ferroelectrics and Sidorkin (2002, 2006) concentrates on the theoretical treatment of phenomenological models of various problems of domain-structure studies. The main concepts of domain structures of ferroic materials are explained in the book by Wadhawan (2000) and in a review by Schranz (1995). Ferroelastic domain structures are reviewed in Boulesteix (1984) and Wadhawan (1991), and are treated in detail by Salje (1990, 1991, 2000*a,b*). The main properties of ferroelectric domain structures are explained in older books or reviews on ferroelectric crystals: Känzig (1957), Jona & Shirane (1962), Fatuzzo & Merz (1967), Mitsui *et al.* (1976), Lines & Glass (1977), Smolenskii *et al.* (1984), Zheludev (1988) and Strukov & Levanyuk (1998). Recent books and reviews on ferroic materials rarely contain new, informed and unifying views on admirable experimental achievements in this field. Applications of ferroelectrics are also described in now older books by Xu (1991) and Uchino (2000). Principles and technical aspects of ferroelectric memories were reviewed by Scott (1998, 2000).

3.4.2. Domain states

3.4.2.1. Principal and basic domain states

As for all crystalline materials, domain structures can be approached in two ways: In the *microscopic description*, a crystal is treated as a regular arrangement of atoms. Domains differ in tiny differences of atomic positions which can be determined only indirectly, *e.g.* by diffraction techniques. In what follows, we shall pay main attention to the *continuum description*, in which a crystal is treated as an anisotropic continuum. Then the crystal properties are described by property tensors (see Section 1.1.1) and the crystal symmetry is expressed by crystallographic point groups. In this approach, domains exhibit different tensor properties that enable one to visualize domains by optical or other methods.

The domain structure observed in a microscope appears to be a patchwork of homogeneous regions – domains – that have various colours and shapes (see Fig. 3.4.1.1). Indeed, the usual description considers a domain structure as a collection of domains and contact regions of domains called domain walls. Strictly speaking, by a *domain* \mathbf{D}_i one understands a connected part of the crystal, called the *domain region*, which is filled with a

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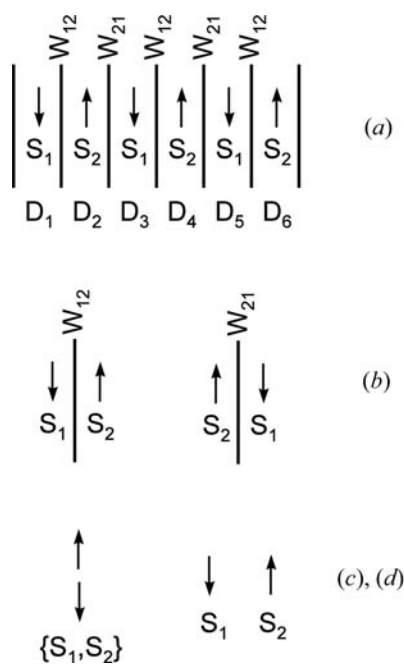


Fig. 3.4.2.1. Hierarchy in domain-structure analysis. (a) Domain structure consisting of domains $\mathbf{D}_1, \mathbf{D}_2, \dots, \mathbf{D}_6$ and domain walls \mathbf{W}_{12} and \mathbf{W}_{21} ; (b) domain twin and reversed twin (with reversed order of domain states); (c) domain pair consisting of two domain states \mathbf{S}_1 and \mathbf{S}_2 ; (d) domain states \mathbf{S}_1 and \mathbf{S}_2 .

homogeneous low-symmetry crystal structure. *Domain walls* can be associated with the boundaries of domain regions. The interior homogeneous bulk structure within a domain region will be called a *domain state*. Equivalent terms are *variant* or *structural variant* (Van Tendeloo & Amelinckx, 1974). We shall use different adjectives to specify domain states. In the microscopic description, domain states associated with the primary order parameter will be referred to as *primary (microscopic, basic) domain states*. Corresponding domain states in the macroscopic description will be called *principal domain states*, which correspond to Aizu's *orientation states*. (An exact definition of principal domain states is given below.)

Further useful division of domain states is possible (though not generally accepted): Domain states that are specified by a constant value of the spontaneous strain are called *ferroelastic domain states*; similarly, *ferroelectric domain states* exhibit constant spontaneous polarization *etc.* Domain states that differ in some tensor properties are called *ferroic* or *tensorial domain states etc.* If no specification is given, the statements will apply to any of these domain states.

A domain \mathbf{D}_i is specified by a domain state \mathbf{S}_j and by domain region \mathcal{Q}_k : $\mathbf{D}_i = \mathbf{D}_i(\mathbf{S}_j, \mathcal{Q}_k)$. Different domains may possess the same domain state but always differ in the domain region that specifies their shape and position in space.

The term 'domain' has also often been used for a domain state. Clear distinction of these two notions is essential in further considerations and is illustrated in Fig. 3.4.2.1. A ferroelectric domain structure (Fig. 3.4.2.1a) consists of six ferroelectric domains $\mathbf{D}_1, \mathbf{D}_2, \dots, \mathbf{D}_6$ but contains only two domain states $\mathbf{S}_1, \mathbf{S}_2$ characterized by opposite directions of the spontaneous polarization depicted in Fig. 3.4.2.1(d). Neighbouring domains have different domain states but non-neighbouring domains may possess the same domain state. Thus domains with odd serial number have the domain state \mathbf{S}_1 (spontaneous polarization 'down'), whereas domains with even number have domain state \mathbf{S}_2 (spontaneous polarization 'up').

A great diversity of observed domain structures are connected mainly with various dimensions and shapes of domain regions, whose shapes depend sensitively on many factors (kinetics of the

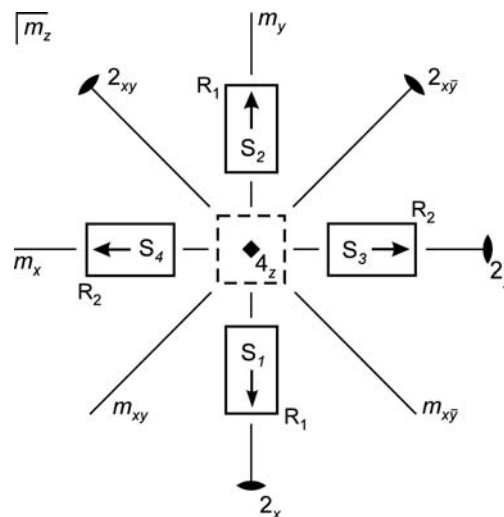


Fig. 3.4.2.2. Exploded view of single-domain states $\mathbf{S}_1, \mathbf{S}_2, \mathbf{S}_3$ and \mathbf{S}_4 (solid rectangles with arrows of spontaneous polarization) formed at a phase transition from a parent phase with symmetry $G = 4_z/m_z m_x m_{xy}$ to a ferroic phase with symmetry $F_1 = 2_x m_y m_z$. The parent phase is represented by a dashed square in the centre with the symmetry elements of the parent group $G = 4_z/m_z m_x m_{xy}$ shown.

phase transition, local stresses, defects *etc.*) It is, therefore, usually very difficult to interpret in detail a particular observed domain pattern. Domain states of domains are, on the other hand, governed by simple laws, as we shall now demonstrate.

We shall consider a ferroic phase transition with a symmetry lowering from a parent (prototypic, high-symmetry) phase with symmetry described by a point group G to a ferroic phase with the point-group symmetry F_1 , which is a subgroup of G . We shall denote this dissymmetrization by a group-subgroup symbol $G \supset F_1$ (or $G \Downarrow F_1$ in Section 3.1.3) and call it a *symmetry descent, dissymmetrization, symmetry lowering* or *reduction*.

As an illustrative example, we choose a phase transition with parent symmetry $G = 4_z/m_z m_x m_{xy}$ and ferroic symmetry $F_1 = 2_x m_y m_z$ (see Fig. 3.4.2.2). Strontium bismuth tantalate (SBT) crystals, for instance, exhibit a phase transition with this symmetry descent (Chen *et al.*, 2000). Symmetry elements in the symbols of G and F_1 are supplied with subscripts specifying the orientation of the symmetry elements with respect to the reference coordinate system. The necessity of this extended notation is exemplified by the fact that the group $G = 4_z/m_z m_x m_{xy}$ has six subgroups with the same 'non-oriented' symbol $mm2$: $m_x m_y 2_z, 2_x m_y m_z, m_x 2_y m_z, m_{xy} m_{xy} 2_z, 2_{xy} m_{xy} m_z, m_{xy} 2_{xy} m_z$. Lower indices thus specify these subgroups unequivocally and the example illustrates an important rule of domain-structure analysis: *All symmetry operations, groups and tensor components must be related to a common reference coordinate system and their orientation in space must be clearly specified.*

The physical properties of crystals in the continuum description are expressed by property tensors. As explained in Section 1.1.4, the crystal symmetry reduces the number of independent components of these tensors. Consequently, for each property tensor the number of independent components in the low-symmetry ferroic phase is the same or higher than in the high-symmetry parent phase. Those tensor components or their linear combinations that are zero in the high-symmetry phase and nonzero in the low-symmetry phase are called *morphic tensor components* or *tensor parameters* and the quantities that appear only in the low-symmetry phase are called *spontaneous quantities* (see Section 3.1.3.2). The morphic tensor components and spontaneous quantities thus reveal the difference between the high- and low-symmetry phases. In our example, the symmetry $F_1 = 2_x m_y m_z$ allows a nonzero spontaneous polarization $\mathbf{P}_0^{(f)} = (P, 0, 0)$, which must be zero in the high-symmetry phase with $G = 4_z/m_z m_x m_{xy}$.

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We shall now demonstrate in our example that the symmetry lowering at the phase transition leads to the existence of several equivalent variants (domain states) of the low-symmetry phase. In Fig. 3.4.2.2, the parent high-symmetry phase is represented in the middle by a dashed square that is a projection of a square prism with symmetry $4_z/m_x m_y m_z$. A possible variant of the low-symmetry phase can be represented by an oblong prism with a vector representing the spontaneous polarization. In Fig. 3.4.2.2, the projection of this oblong prism is drawn as a rectangle which is shifted out of the centre for better recognition. We denote by \mathbf{S}_1 a homogeneous low-symmetry phase with spontaneous polarization $\mathbf{P}_0^{(1)} = (P, 0, 0)$ and with symmetry $F_1 = 2_x m_y m_z$. Let us, mentally, increase the temperature to above the transition temperature and then apply to the high-symmetry phase an operation 2_z , which is a symmetry operation of this high-symmetry phase but not of the low-symmetry phase. Then decrease the temperature to below the transition temperature. The appearance of another variant of the low-symmetry phase \mathbf{S}_2 with spontaneous polarization $\mathbf{P}_0^{(2)} = (-P, 0, 0)$ obviously has the same probability of appearing as had the variant \mathbf{S}_1 . Thus the two variants of the low-symmetry phase \mathbf{S}_1 and \mathbf{S}_2 can appear with the same probability if they are related by a symmetry operation suppressed (lost) at the transition, *i.e.* an operation that was a symmetry operation of the high-symmetry phase but is not a symmetry operation of the low-symmetry phase \mathbf{S}_1 . In the same way, the lost symmetry operations 4_z and 4_z^3 generate from \mathbf{S}_1 two other variants, \mathbf{S}_3 and \mathbf{S}_4 , with spontaneous polarizations $(0, P, 0)$ and $(0, -P, 0)$, respectively. Variants of the low-symmetry phase that are related by an operation of the high-symmetry group G are called *crystallographically equivalent (in G) variants*. Thus we conclude that *crystallographically equivalent (in G) variants of the low-symmetry phase have the same chance of appearing*.

We shall now make similar considerations for a general ferroic phase transition with a symmetry descent $G \supset F_1$. By the *state \mathbf{S} of a crystal* we shall understand, in the continuum description, the set of all its properties expressed by property (matter) tensors in the reference Cartesian crystallophysical coordinate system of the parent phase (see Example 3.2.3.9 in Section 3.2.3.3.1). A state defined in this way may change not only with temperature and external fields but also with the orientation of the crystal in space.

We denote by \mathbf{S}_1 a state of a homogeneous ferroic phase. If we apply to \mathbf{S}_1 a symmetry operation g_i of the group G , then the ferroic phase in a new orientation will have the state \mathbf{S}_j , which may be identical with \mathbf{S}_1 or different. Using the concept of group action (explained in detail in Section 3.2.3.3.1) we express this operation by a simple relation:

$$g_j \mathbf{S}_1 = \mathbf{S}_j, \quad g_j \in G. \quad (3.4.2.1)$$

Let us first turn our attention to operations $f_j \in G$ that do not change the state \mathbf{S}_1 :

$$f_j \mathbf{S}_1 = \mathbf{S}_1, \quad f_j \in G. \quad (3.4.2.2)$$

The set of all operations of G that leave \mathbf{S}_1 invariant form a group called a *stabilizer (or isotropy group)* of a state \mathbf{S}_1 in the group G . This stabilizer, denoted by $I_G(\mathbf{S}_1)$, can be expressed explicitly in the following way:

$$I_G(\mathbf{S}_1) \equiv \{g \in G | g \mathbf{S}_1 = \mathbf{S}_1\}, \quad (3.4.2.3)$$

where the right-hand part of the equation should be read as ‘a set of all operations of G that do not change the state \mathbf{S}_1 ’ (see Section 3.2.3.3.2).

Here we have to explain the difference between the concept of a stabilizer of an object and the symmetry of that object. By the *symmetry group F of an object* one understands the set of all operations (isometries) that leave this object \mathbf{S} invariant. The symmetry group F of an object is considered to be an inherent

property that does not depend on the orientation and position of the object in space. (The term *eigensymmetry* is used in Chapter 3.3 for symmetry groups defined in this way. Another expression is *non-oriented symmetry*.) In this case, the symmetry elements of F are ‘attached’ to the object.

A stabilizer describes the symmetry properties of an object in another way, in which the object and the group of isometries are decoupled. One is given a group G , the symmetry elements of which have a defined orientation in a fixed reference system. The object can have any orientation in this reference system. Those operations of G that map the object in a given orientation onto itself form the *stabilizer $I_G(\mathbf{S}_1)$ of \mathbf{S}_1 in the group G* . In this case, the stabilizer depends on the orientation of the object in space and is expressed by an ‘oriented’ group symbol F_1 with subscripts defining the orientation of the symmetry elements of F_1 . Only for certain ‘prominent’ orientations will the stabilizer acquire a symmetry group of the same crystal class (crystallographic point group) as the *eigensymmetry* of the object.

We shall define a *single-domain orientation* as a prominent orientation of the crystal in which the stabilizer $I_G(\mathbf{S}_1)$ of its state \mathbf{S}_1 is equal to the symmetry group F_1 which is, after removing subscripts specifying the orientation, identical with the *eigensymmetry* of the ferroic phase:

$$I_G(\mathbf{S}_1) = F_1. \quad (3.4.2.4)$$

This equation thus declares that the crystal in the state \mathbf{S}_1 has a prominent single-domain orientation.

The concept of the stabilizer allows us to identify the ‘*eigensymmetry*’ of a domain state (or an object in general) \mathbf{S}_i with the crystallographic class (non-oriented point group) of the stabilizer of this state in the group of all rotations $O(3)$, $I_{O(3)}(\mathbf{S}_i)$.

Since we shall further deal mainly with states of the ferroic phase in single-domain orientations, we shall use the term ‘state’ for a ‘state of the crystal in a single-domain orientation’, unless mentioned otherwise. Then the stabilizer $I_G(\mathbf{S}_1)$ will usually be replaced by the group F_1 , although all statements have been derived and hold for stabilizers.

The difference between symmetry groups of a crystal and stabilizers will become more obvious in the treatment of secondary domain states in Section 3.4.2.2 and in discussing disoriented ferroelastic domain states (see Section 3.4.3.6.3).

As we have seen in our illustrative example, the suppressed operations generate from the first state \mathbf{S}_1 other states. Let g_j be such a *suppressed operation*, *i.e.* $g_j \in G$ but $g_j \notin F_1$. Since all operations that retain \mathbf{S}_1 are collected in F_1 , the operation g_j must transform \mathbf{S}_1 into another state \mathbf{S}_j ,

$$g_j \mathbf{S}_1 = \mathbf{S}_j \neq \mathbf{S}_1, \quad g_j \in G, \quad g_j \notin F_1, \quad (3.4.2.5)$$

and we say that the state \mathbf{S}_j is *crystallographically equivalent (in G) with the state \mathbf{S}_1* , $\mathbf{S}_j \stackrel{G}{\sim} \mathbf{S}_1$.

We define *principal domain states* as crystallographically equivalent (in G) variants of the low-symmetry phase in single-domain orientations that can appear with the same probability in the ferroic phase. They represent possible macroscopic bulk structures of (1) ferroic single-domain crystals, (2) ferroic domains in non-ferroelastic domain structures (see Section 3.4.3.5), or (3) ferroic domains in any ferroic domain structure, if all spontaneous strains are suppressed [this is the so-called parent clamping approximation (PCA), see Section 3.4.2.5]. In what follows, *any statement formulated for principal domain states or for single-domain states applies to any of these three situations*. Principal domain states are in one-to-one correspondence with *orientation states* (Aizu, 1969) or *orientation variants* (Van Tendeloo & Amelinckx, 1974). The adjective ‘principal’ distinguishes these domain states from primary (microscopic, basic – see Section 3.4.2.5) domain states and from degenerate domain states, defined in Section 3.4.2.2, and implies that any two of these

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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 a 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)			

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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

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GI★KoBo-1 and in Kopský (2001). The corresponding Cartesian tensor components are available in Section 1.1.4 and in standard textbooks (e.g. Nye, 1985; Sirotnin & Shaskolskaya, 1982).

(2) If

$$I_G(\tau_a^{(\omega(1))}) = F_1, \quad (3.4.2.39)$$

then any of $m = n_\tau/d_\alpha$ tensorial covariants $\tau_a^{(\omega)}$, $a = 1, 2, \dots, m$, is a possible principal tensor parameter $\varphi^{(1)}$ of the transition $G \supset F_1$. Any two of $n_f = |G| : |F_1|$ principal domain states differ in some, or all, components of these covariants. The principal tensor parameter φ plays a similar symmetric (but generally not thermodynamic) role as the order parameter η does in the Landau theory. Only for equitranslational phase transitions is one of the principal tensor parameters (that with the temperature-dependent coefficient) identical with the primary order parameter of the Landau theory (see Section 3.1.3).

(3) If

$$I_G(\tau_a^{(\omega(1))}) = L_1, \quad F_1 \subset L_1 \subset G, \quad (3.4.2.40)$$

then $\tau_a^{(\omega(1))}$ represents the secondary tensor parameter λ (see Section 3.1.3.2). There exist $n_\lambda = |G| : |L_1|$ secondary domain states $\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_{n_\lambda}$ that differ in λ . Unlike in the two preceding cases (1) and (2), several intermediate groups L_1, M_2, \dots (with secondary tensor parameters λ, μ, \dots) that fulfil condition (3.4.2.40) can exist.

Now we shall indicate how one can find particular property tensors that fulfil conditions (3.4.2.39) or (3.4.2.40). The solution of this group-theoretical task consists of three steps:

(i) For a given point-group symmetry descent $G \supset F_1$, or $G \supset L_1$, one finds the *representation* Γ_η that specifies the *transformation properties of the principal, or secondary, tensor parameter*, which plays the role of the order parameters in a continuum description. This task is called an inverse Landau problem (see Section 3.1.3 for more details). The solution of this problem is available in Tables 3.4.2.7 and 3.1.3.1, in the software *GI★KoBo-1* and in Kopský (2001), where the letters A, B signify one-dimensional irreducible representations, and letters E and T two- and three-dimensional ones. The dimensionality d_η , or d_λ , of the representation Γ_η , or Γ_λ , specifies the maximal number of independent components of the principal, or secondary, tensor parameter φ , or λ , respectively. ‘Reducible’ indicates that Γ_η is a reducible representation.

(ii) In Table 3.1.3.1 one finds in the second column, for a given G and Γ_η , or Γ_λ (first column), the *standard variables* designating in a standardized way the covariant tensor components of the principal, or secondary, tensor parameters (for more details see Section 3.1.3.1 and the manual of the software *GI★KoBo-1*). For two- and three-dimensional irreducible representations, this column contains relations that restrict the values of the components and thus reduce the number of independent components.

(iii) *The association of covariant tensor components* of property tensors *with standard variables* is tabulated for all irreducible representations in an abridged version in Table 3.1.3.1, in the

column headed *Principal tensor parameters*, and in full in the main table of the software *GI★KoBo-1* and of Kopský (2001).

Phase transitions associated with reducible representations are treated in detail only in the software *GI★KoBo-1* and in Kopský (2001). Fortunately, these phase transitions occur rarely in nature.

A rich variety of observed structural phase transitions can be found in Tomaszewski (1992). This database lists 3446 phase transitions in 2242 crystalline materials.

Example 3.4.2.4. Morphic tensor components associated with $4_z/m_z m_x m_{xy} \supset 2_x m_y m_z$ symmetry descent

(1) *Principal tensor parameters* $\varphi^{(1)}$. The representation Γ_η that specifies the transformation properties of the principal tensor parameter $\varphi^{(1)}$ (and for equitranslational phase transitions also the primary order parameter $\eta^{(1)}$) can be found in the first column of Table 3.1.3.1 for $G = 4_z/m_z m_x m_{xy}$ and $F_1 = 2_x m_y m_z$; the R -irreducible representation (R -irep) $\Gamma_\eta = E_u$. Therefore, the principal tensor parameter $\varphi^{(1)}$ (or the primary order parameter $\eta^{(1)}$) has two components $(\varphi_1^{(1)}, \varphi_2^{(1)})$ [or $(\eta_1^{(1)}, \eta_2^{(1)})$]. The standard variables are in the second column: $(x_1^-, 0)$. This means that only the first component $\varphi_1^{(1)}$ (or $\eta_1^{(1)}$) is nonzero. In the column *Principal tensor parameters*, one finds that $\varphi_1^{(1)} = P_1$ (or $\eta_1^{(1)} = P_1$), i.e. one principal tensor parameter is spontaneous polarization and the spontaneous polarization in the first domain state \mathbf{S}_1 is $P_{(s)} = (P, 00)$. Other principal tensor parameters can be found in the software *GI★KoBo-1* or in Kopský (2001), p. 185: $(g_4, 0)$, $(d_{11}, 0)$, $(d_{12}, 0)$, $(d_{13}, 0)$, $(d_{26}, 0)$, $(d_{35}, 0)$ (the physical meaning of the components is explained in Table 3.4.3.5).

(2) *Secondary tensor parameters* $\lambda^{(1)}, \mu^{(1)}, \dots$

In the group lattice (group–subgroup chains) in Fig. 3.1.3.1, one finds that the only intermediate group between $4_z/m_z m_x m_{xy}$ and $2_x m_y m_z$ is $L_1 = m_x m_y m_z$. In the same table of the software *GI★KoBo-1* or in Kopský (2001), one finds $\Gamma_\lambda = B_{1g}$ and the following one-dimensional secondary tensor parameters: $u_1 - u_2$; $A_{14} + A_{25}$, A_{36} ; $s_{11} - s_{22}$, $s_{13} - s_{23}$, $s_{44} - s_{55}$; $Q_{11} - Q_{22}$, $Q_{12} - Q_{21}$, $Q_{13} - Q_{23}$, $Q_{31} - Q_{32}$, $Q_{44} - Q_{55}$.

The use of covariant tensor components has two practical advantages:

Firstly, the change of tensor components at a ferroic phase transition is completely described by the appearance of new nonzero covariant tensor components. If needed, Cartesian tensor components corresponding to covariant components can be calculated by means of *conversion equations*, which express Cartesian tensor components as linear combinations of covariant tensor components [for details on tensor covariants and conversion equations see the manual and Appendix E of the software *GI★KoBo-1* and Kopský (2001)].

Secondly, calculation of property tensors in various domain states is substantially simplified: transformations of Cartesian tensor components, which are rather involved for higher-rank tensors, are replaced by a simpler transformation of covariant tensor components by matrices $D^{(n)}$ of the matrix representation of Γ_η , or of Γ_λ [see again the software *GI★KoBo-1* and Kopský

Table 3.4.2.4. *Morphic properties, tensor parameters, order parameters and domain states*

T, U, S, V: property tensors; TOP: designation of tensor or order parameter; Γ : representation of G expressing the transformation properties of TOP. The terms ‘full’ and ‘partial’ were introduced by Aizu (1970a).

Morphic property	TOP	Γ	Stabilizer of TOP	Domain states
Spontaneous components of tensor T	φ	Γ_φ	F_1	Principal (full) in tensor T
Spontaneous components of tensor U	ψ	Γ_ψ	F_1	Principal (full) in tensor U
Spontaneous components of tensor S	σ	Γ_σ	F_1	Principal (full) in tensor S
Spontaneous components of tensor V	λ	Γ_λ	$L_1, F_1 \subset L_1 \subset G$	Degenerate (partial) in tensor V
Primary order parameter	η	Γ_η	\mathcal{F}_1	Basic (microscopic)
Pseudoproper order parameter	ζ	Γ_η	\mathcal{F}_1	Basic (microscopic)
Secondary (improper) order parameter	ξ	Γ_ξ	$\mathcal{L}_1, \mathcal{F}_1 \subset \mathcal{L}_1 \subset \mathcal{G}$	Secondary (improper) microscopic

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(2001)]. The determination of the tensor properties of all domain states is discussed in full in the book by Kopský (1982).

The relations between morphic properties, tensor parameters, order parameters and names of domain states are summarized in Table 3.4.2.4. Macroscopic principal domain states can be distinguished by various property tensors that transform either according to the same representation Γ_φ (tensors T and U) or different representations Γ_φ and Γ_σ (tensors T and S). In the microscopic description, a basic domain state may sometimes be shared by two physically different order parameters: a primary order parameter η (the order parameter, components of which form a quadratic invariant with a temperature-dependent coefficient in the free energy) and a pseudoproper order parameter ζ that transforms according to the same representation Γ_η as the primary order parameter but has a temperature coefficient that is almost independent of temperature. This is, however, rather rare (see, e.g., Tolédano & Dmitriev, 1996).

3.4.2.4. Synoptic table of ferroic transitions and domain states

The considerations of this and all following sections can be applied to any phase transition with point-group symmetry descent $G \supset F$. All such non-magnetic *crystallographically non-equivalent symmetry descents* are listed in Table 3.4.2.7 together with some other data associated with symmetry reduction at a ferroic phase transition. These symmetry descents can also be traced in lattices of subgroups of crystallographic point groups, which are displayed in Figs. 3.1.3.1 and 3.1.3.2.

The symmetry descents $G \supset F_1$ listed in Table 3.4.2.7 are analogous to Aizu's 'species' (Aizu, 1970a), in which the symbol F stands for the symbol \supset in our symmetry descent, and the orientation of symmetry elements of the group F_1 with respect to G is specified by letters p, s, ps, pp etc. A list of 212 non-ferro-

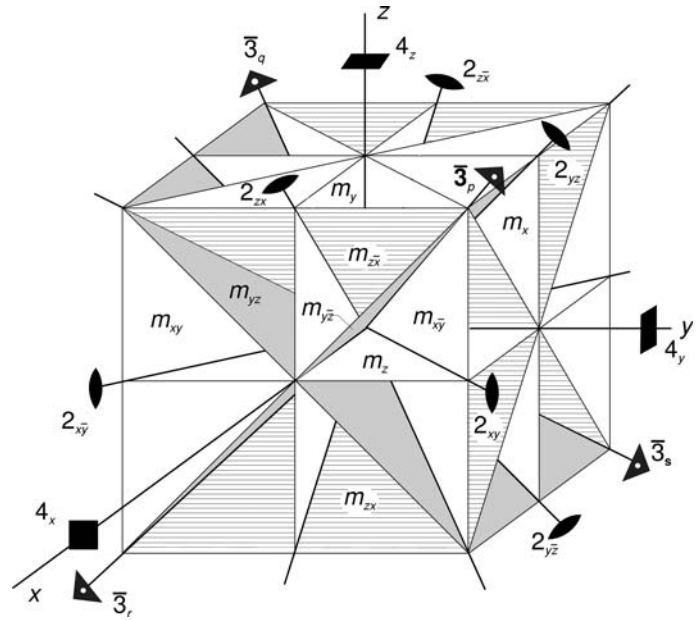


Fig. 3.4.2.3. Oriented symmetry operations of the cubic group $m\bar{3}m$ and of its subgroups. The Cartesian (rectangular) coordinate system x, y, z is identical with the crystallographic and crystallophysical coordinate systems. Correlation with other notations is given in Table 3.4.2.5.

magnetic species together with their property tensors is available online (Janovec, 2012).

As we have already stated, any systematic analysis of domain structures requires an unambiguous specification of the orientation and location of symmetry elements in space. Moreover, in a continuum approach, the description of crystal properties is performed in a rectangular (Cartesian) coordinate system, which

Table 3.4.2.5. Symbols of symmetry operations of the point group $m\bar{3}m$

Standard: symbols used in Section 3.1.3, in the present chapter and in the software; all symbols refer to the cubic crystallographic (Cartesian) basis, $p \equiv [111]$ (all positive), $q \equiv [\bar{1}\bar{1}\bar{1}]$, $r \equiv [11\bar{1}]$, $s \equiv [\bar{1}\bar{1}1]$. BC: Bradley & Cracknell (1972). AH: Altmann & Herzog (1994). IT A: IT A (2005). Jones: Jones' faithful representation symbols express the action of a symmetry operation on a vector (xyz) (see e.g. Bradley & Cracknell, 1972).

Standard	BC	AH	IT A	Jones	Standard	BC	AH	IT A	Jones
1 or e	E	E	1	x, y, z	$\bar{1}$ or i	I	i	$\bar{1}$ 0, 0, 0	$\bar{x}, \bar{y}, \bar{z}$
2_z	C_{2z}	C_{2z}	2 0, 0, z	\bar{x}, \bar{y}, z	m_z	σ_z	σ_z	m $x, y, 0$	x, y, \bar{z}
2_x	C_{2x}	C_{2x}	2 $x, 0, 0$	x, \bar{y}, \bar{z}	m_x	σ_x	σ_x	m 0, y, z	\bar{x}, y, z
2_y	C_{2y}	C_{2y}	2 0, $y, 0$	\bar{x}, y, \bar{z}	m_y	σ_y	σ_y	m $x, 0, z$	x, \bar{y}, z
2_{xy}	C_{2a}	C'_{2a}	2 $x, x, 0$	y, x, \bar{z}	m_{xy}	σ_{da}	σ_{d1}	m x, \bar{x}, z	\bar{y}, \bar{x}, z
$2_{x\bar{y}}$	C_{2b}	C'_{2b}	2 $x, \bar{x}, 0$	$\bar{y}, \bar{x}, \bar{z}$	$m_{x\bar{y}}$	σ_{db}	σ_{d2}	m x, x, z	y, x, z
2_{zx}	C_{2c}	C'_{2c}	2 $x, 0, x$	z, \bar{y}, x	m_{zx}	σ_{dc}	σ_{d3}	m \bar{x}, y, x	\bar{z}, y, \bar{x}
$2_{z\bar{x}}$	C_{2e}	C'_{2e}	2 $\bar{x}, 0, x$	$\bar{z}, \bar{y}, \bar{x}$	$m_{z\bar{x}}$	σ_{de}	σ_{d5}	m x, y, x	z, y, x
2_{yz}	C_{2d}	C'_{2d}	2 0, y, y	\bar{x}, z, y	m_{yz}	σ_{dd}	σ_{d4}	m x, y, \bar{y}	x, \bar{z}, \bar{y}
$2_{y\bar{z}}$	C_{2f}	C'_{2f}	2 0, y, \bar{y}	$\bar{x}, \bar{z}, \bar{y}$	$m_{y\bar{z}}$	σ_{df}	σ_{d6}	m x, y, y	x, z, y
3_p	C_{31}^+	C_{31}^+	3^+ x, x, x	z, x, y	$\bar{3}_p$	S_{61}^-	S_{61}^-	$\bar{3}^+$ x, x, x	$\bar{z}, \bar{x}, \bar{y}$
3_q	C_{32}^+	C_{32}^+	3^+ \bar{x}, \bar{x}, x	\bar{z}, x, \bar{y}	$\bar{3}_q$	S_{62}^-	S_{62}^-	$\bar{3}^+$ \bar{x}, \bar{x}, x	z, \bar{x}, y
3_r	C_{33}^+	C_{33}^+	3^+ x, \bar{x}, \bar{x}	\bar{z}, \bar{x}, y	$\bar{3}_r$	S_{63}^-	S_{63}^-	$\bar{3}^+$ x, \bar{x}, \bar{x}	z, x, \bar{y}
3_s	C_{34}^+	C_{34}^+	3^+ \bar{x}, x, \bar{x}	z, \bar{x}, \bar{y}	$\bar{3}_s$	S_{64}^-	S_{64}^-	$\bar{3}^+$ \bar{x}, x, \bar{x}	\bar{z}, x, y
3_p^2	C_{31}^-	C_{31}^-	3^- x, x, x	y, z, x	$\bar{3}_p^5$	S_{61}^+	S_{61}^+	$\bar{3}^-$ x, x, x	$\bar{y}, \bar{z}, \bar{x}$
3_q^2	C_{32}^-	C_{32}^-	3^- \bar{x}, \bar{x}, x	y, \bar{z}, \bar{x}	$\bar{3}_q^5$	S_{62}^+	S_{62}^+	$\bar{3}^-$ \bar{x}, \bar{x}, x	\bar{y}, z, x
3_r^2	C_{33}^-	C_{33}^-	3^- x, \bar{x}, \bar{x}	\bar{y}, z, \bar{x}	$\bar{3}_r^5$	S_{63}^+	S_{63}^+	$\bar{3}^-$ x, \bar{x}, \bar{x}	y, \bar{z}, x
3_s^2	C_{34}^-	C_{34}^-	3^- \bar{x}, x, \bar{x}	\bar{y}, \bar{z}, x	$\bar{3}_s^5$	S_{64}^+	S_{64}^+	$\bar{3}^-$ \bar{x}, x, \bar{x}	y, z, \bar{x}
4_z	C_{4z}^+	C_{4z}^+	4^+ 0, 0, z	\bar{y}, x, z	$\bar{4}_z$	S_{4z}^-	S_{4z}^-	$\bar{4}^+$ 0, 0, z	y, \bar{x}, \bar{z}
4_x	C_{4x}^+	C_{4x}^+	4^+ $x, 0, 0$	x, \bar{z}, y	$\bar{4}_x$	S_{4x}^-	S_{4x}^-	$\bar{4}^+$ $x, 0, 0$	\bar{x}, z, \bar{y}
4_y	C_{4y}^+	C_{4y}^+	4^+ 0, $y, 0$	z, y, \bar{x}	$\bar{4}_y$	S_{4y}^-	S_{4y}^-	$\bar{4}^+$ 0, $y, 0$	\bar{z}, \bar{y}, x
4_z^3	C_{4z}^-	C_{4z}^-	4^- 0, 0, z	y, \bar{x}, z	$\bar{4}_z^3$	S_{4z}^+	S_{4z}^+	$\bar{4}^-$ 0, 0, z	\bar{y}, x, \bar{z}
4_x^3	C_{4x}^-	C_{4x}^-	4^- $x, 0, 0$	x, z, \bar{y}	$\bar{4}_x^3$	S_{4x}^+	S_{4x}^+	$\bar{4}^-$ $x, 0, 0$	\bar{x}, \bar{z}, y
4_y^3	C_{4y}^-	C_{4y}^-	4^- 0, $y, 0$	\bar{z}, y, x	$\bar{4}_y^3$	S_{4y}^+	S_{4y}^+	$\bar{4}^-$ 0, $y, 0$	z, \bar{y}, \bar{x}

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differs in hexagonal and trigonal crystals from the crystallographic coordinate system common in crystallography. Last but not least, a ready-to-use and user-friendly presentation calls for symbols that are explicit and concise.

To meet these requirements, we use in this chapter, in Section 3.1.3 and in the software *GI★KoBo-1* a symbolism in which the orientations of crystallographic elements and operations are expressed by means of suffixes related to a reference Cartesian coordinate system. The relation of this reference Cartesian coordinate system – called a *crystallophysical coordinate system* – to the usual crystallographic coordinate system is a matter of convention. We adhere to the generally accepted rules [see Nye (1985) Appendix B, Sirotnin & Shaskolskaya (1982), Shuvalov (1988), and *IEEE Standards on Piezoelectricity*, 1987].

We list all symbols of crystallographic symmetry operations and a comparison of these symbols with other notations in Tables 3.4.2.5 and 3.4.2.6 and in Figs. 3.4.2.3 and 3.4.2.4.

Now we can present the synoptic Table 3.4.2.7.

3.4.2.4.1. Explanation of Table 3.4.2.7

G : point group expressing the *symmetry of the parent (prototypic) phase*. Subscripts of generators in the group symbol specify their orientation in the Cartesian (rectangular) crystallophysical coordinate system of the group G (see Tables 3.4.2.5 and 3.4.2.6, and Figs. 3.4.2.3 and 3.4.2.4).

F_1 : this point group is a proper subgroup of G given in the first column and expresses the *symmetry of the ferroic phase in the first single-domain state* S_1 . In accordance with *IT A* (2005), five groups are given in two orientations (bold and normal type). Subscripts of generators in the group symbol specify their orientation in the Cartesian (rectangular) crystallophysical coordinate system of the group G (see Tables 3.4.2.5 and 3.4.2.6, and Figs. 3.4.2.3 and 3.4.2.4). In the cubic groups, the direction of the body diagonal is denoted by abbreviated symbols: $p \equiv [111]$ (all positive), $q \equiv [\bar{1}\bar{1}\bar{1}]$, $r \equiv [1\bar{1}\bar{1}]$, $s \equiv [\bar{1}\bar{1}1]$. In the hexagonal and trigonal groups, axes x' , y' and x'' , y'' of a Cartesian coordinate system are rotated about the z axis through 120° and 240° , respectively, from the crystallophysical Cartesian coordinate axes x and y .

Symmetry groups in parentheses are groups conjugate to F_1 under G (see Section 3.2.3.2). These are symmetry groups (stabilizers) of some domain states S_k different from S_1 (for more details see Section 3.4.2.2.3).

Γ_η : *physically irreducible representation of the group* G . This specifies the transformation properties of the principal tensor parameter of the phase transition in a continuum description and transformation properties of the primary order parameter η

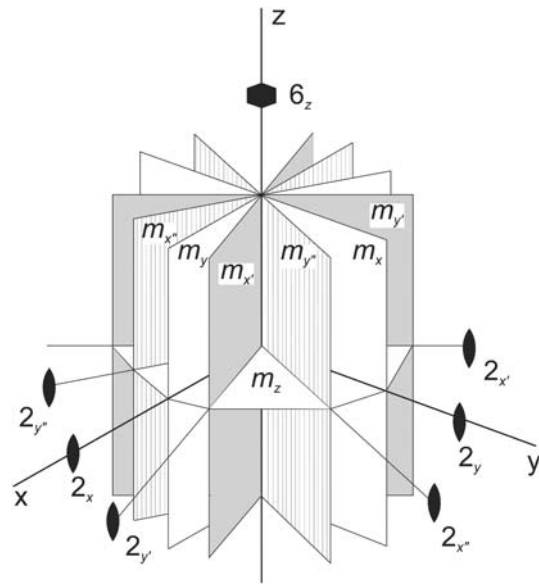


Fig. 3.4.2.4. Oriented symmetry operations of the hexagonal group $6/mmm$ and of its hexagonal and trigonal subgroups. The coordinate system x, y, z corresponds to the Cartesian crystallophysical coordinate system, the axes x, y, z of the crystallographic coordinate system are parallel to the twofold rotation axes $2_x, 2_y$ and to the sixfold rotation axis 6_z . Correlation with other notations is given in Table 3.4.2.6.

of the *equitranslational* phase transitions in the microscopic description. The letters A, B signify one-dimensional representations, and letters E and T two- and three-dimensional irreducible representations, respectively. Two letters T indicate that the symmetry descent $G \subset F_1$ can be accomplished by two non-equivalent three-dimensional irreducible representations (see Table 3.1.3.2). ‘Reducible’ denotes a reducible representation of G . In this case, there are always several non-equivalent reducible representations inducing the same descent $G \subset F_1$ [for more detailed information see the software *GI★KoBo-1* and Kopský (2001)].

Knowledge of Γ_η enables one to determine for all ferroic transitions property tensors and their components that are different in all principal domain states, and, for equitranslational transitions only, microscopic displacements and/or ordering of atoms and molecules that are different in different basic (microscopic) domain states (for details see Section 3.1.3, especially Table 3.1.3.1, and Section 3.1.2).

$N_G(F_1)$: the *normalizer of* F_1 in G (defined in Section 3.2.3.2.4) determines subgroups conjugate to F_1 in G and specifies which

Table 3.4.2.6. Symbols of symmetry operations of the point group $6/mmm$

Standard: symbols used in Section 3.1.3, in the present chapter and in the software; suffixes (in italic) refer to the Cartesian crystallophysical coordinate system. BC: Bradley & Cracknell (1972). AH: Altmann & Herzig (1994). *IT A*: *IT A* (2005), coordinates (in Sans Serif) are expressed in a crystallographic hexagonal basis. Jones: Jones’ faithful representation symbols express the action of a symmetry operation of a vector (xyz) in a crystallographic basis (see e.g. Bradley & Cracknell, 1972).

Standard	BC	AH	<i>IT A</i>	Jones	Standard	BC	AH	<i>IT A</i>	Jones
1 or e	E	E	1	x, y, z	$\bar{1}$ or i	I	I	$\bar{1}$ 0, 0, 0	$\bar{x}, \bar{y}, \bar{z}$
6_z	C_6^+	C_6^+	6^+ 0, 0, z	$x - y, x, z$	$\bar{6}_z$	S_3^-	S_3^-	$\bar{6}^+$ 0, 0, z	$y - x, \bar{x}, \bar{z}$
3_z	C_3^+	C_3^+	3^+ 0, 0, z	$\bar{y}, x - y, z$	$\bar{3}_z$	S_6^-	S_6^-	$\bar{3}^+$ 0, 0, z	$y, y - x, \bar{z}$
2_z	C_2	C_2	2 0, 0, z	\bar{x}, \bar{y}, z	m_z	σ_h	σ_h	m $x, y, 0$	x, y, \bar{z}
3_z^2	C_3^-	C_3^-	3^- 0, 0, z	$y - x, \bar{x}, z$	$\bar{3}_z^5$	S_6^+	S_6^+	$\bar{3}^-$ 0, 0, z	$x - y, x, \bar{z}$
6_z^5	C_6^-	C_6^-	6^- 0, 0, z	$y, y - x, z$	$\bar{6}_z^5$	S_3^+	S_3^+	$\bar{6}^-$ 0, 0, z	$\bar{y}, x - y, \bar{z}$
2_x	C_{21}''	C_{21}''	2 $x, 0, 0$	$x - y, \bar{y}, \bar{z}$	m_x	σ_{v1}	σ_{v1}	m $x, 2x, z$	$y - x, y, z$
$2_{x'}$	C_{22}''	C_{22}''	2 $0, y, 0$	$\bar{x}, y - x, \bar{z}$	$m_{x'}$	σ_{v2}	σ_{v2}	m $2x, x, z$	$x, x - y, z$
$2_{x''}$	C_{23}''	C_{23}''	2 $x, x, 0$	y, x, \bar{z}	$m_{x''}$	σ_{v3}	σ_{v3}	m x, \bar{x}, z	\bar{y}, \bar{x}, z
2_y	C_{21}'	C_{21}'	2 $x, 2x, 0$	$y - x, y, \bar{z}$	m_y	σ_{d1}	σ_{d1}	m $x, 0, z$	$x - y, \bar{y}, z$
$2_{y'}$	C_{22}'	C_{22}'	2 $2x, x, 0$	$x, x - y, \bar{z}$	$m_{y'}$	σ_{d2}	σ_{d2}	m $0, y, z$	$\bar{x}, y - x, z$
$2_{y''}$	C_{23}'	C_{23}'	2 $x, \bar{x}, 0$	$\bar{y}, \bar{x}, \bar{z}$	$m_{y''}$	σ_{d3}	σ_{d3}	m x, x, z	y, x, z

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domain states have the same symmetry (stabilizer in G). The number n_F of subgroups conjugate to F_1 in G is $n_F = [G : N_G(F_1)] = |G| : |N_G(F_1)|$ [see equation (3.4.2.36)] and the number d_F of principal domain states with the same symmetry is $d_F = [N_G(F_1) : F_1] = |N_G(F_1)| : |F_1|$ [see equation (3.4.2.35)]. There are three possible cases:

(i) $N_G(F_1) = G$. There are no subgroups conjugate to F_1 and the symmetry group F_i (stabilizer of \mathbf{S}_i in G) of all principal domain states $\mathbf{S}_1, \mathbf{S}_2, \dots, \mathbf{S}_n$ is equal to F_i for all $i = 1, 2, \dots, n$; hence domain states cannot be distinguished by their symmetry. The group F_1 is a normal subgroup of G , $F_1 \triangleleft G$ (see Section 3.2.3.2). This is always the case if there are just two single-domain states $\mathbf{S}_1, \mathbf{S}_2$, i.e. if the index of F_1 in G equals two, $[G : F_1] = |G| : |F_1| = 2$.

(ii) $N_G(F_1) = F_1$. Then any two domain states $\mathbf{S}_i, \mathbf{S}_k$ have different symmetry groups (stabilizers), $\mathbf{S}_i \neq \mathbf{S}_k \Leftrightarrow F_i \neq F_k$, i.e. there is a one-to-one correspondence between single-domain states and their symmetries, $\mathbf{S}_i \Leftrightarrow F_i$. In this case, principal domain states \mathbf{S}_i can be specified by their symmetries F_i , $i = 1, 2, \dots, n$. The number n_F of different groups conjugate to F_1 is equal to the index $[G : F_1] = |G| : |F_1| = n$.

(iii) $F_1 \subset N_G(F_1) \subset G$. Some, but not all, domain states $\mathbf{S}_i, \mathbf{S}_k$ have identical symmetry groups (stabilizers) $F_i = F_k$. The number d_F of domain states with the same symmetry group is $d_F = [N_G(F_1) : F_1] = |N_G(F_1)| : |F_1|$ [see equation (3.4.2.35)], $1 < d_F < n$. The number n_F of different groups conjugate to F_1 is equal to the index $n_F = [G : N_G(F_1)] = |G| : |N_G(F_1)|$ [see equation (3.4.2.36)] and in this case $1 < n_F < n$. It always holds that $n_F d_F = n$ [see equation (3.4.2.37)].

$K_G(F_1, g_{1j})$: *twinning group of a domain pair* ($\mathbf{S}_1, \mathbf{S}_j$). This group is defined in Section 3.4.3.2. It can be considered a colour (polychromatic) group involving c colours, where $c = [K_{1j} : F_1]$, and is, therefore, defined by *two* groups K_{1j} and F_1 , and its full symbol is $K_{1j}(F_1)$. In this column only K_{1j} is given, since F_1 appears in the second column of the table.

If the group symbol of K_{1j} contains generators with the star symbol, *, which signifies transposing operations of the domain pair ($\mathbf{S}_1, \mathbf{S}_j$), then the symbol $K_{1j}(F_1)$ denotes a dichromatic ('black-and-white') group signifying a completely transposable domain pair. In this special case, just the symbol K_{1j} containing stars * specifies the group F_1 unequivocally.

The number in parentheses after the group symbol of K_{1j} is equal to the number of twinning groups K_{1k} equivalent with K_{1j} .

In the continuum description, a twinning group is significant in at least in two instances:

(1) A twinning group $K_{1j}(F_1)$ specifies the distinction of two domain states \mathbf{S}_1 and $\mathbf{S}_j = g_{1j}\mathbf{S}_1$, where $g_{1j} \in G$ (see Sections 3.4.3.2 and 3.4.3.4).

(2) A twinning group $K_{1j}(F_1)$ may assist in signifying classes of equivalent domain pairs (orbits of domain pairs). In most cases, to a twinning group F_{1j} there corresponds just one class of equivalent domain pairs (an orbit) $G(\mathbf{S}_1, \mathbf{S}_j)$; then a twinning group can represent this class of equivalent domain pairs. Nevertheless, in some cases two or more classes of equivalent domain pairs have a common twinning group. Then one has to add a switching operation g_{1j} to the twinning group, $K_{1j}(F_1, g_{1j})$ (see the end of Section 3.4.3.2). In this way, classes of equivalent domain pairs $G(\mathbf{S}_1, \mathbf{S}_j)$ are denoted in synoptic Tables 3.4.2.7 and 3.4.3.6.

Twinning groups given in column K_{1j} thus specify *all G-orbits of domain pairs*. The number of G -orbits and representative domain pairs for each orbit are determined by double cosets of group F_1 (see Section 3.4.3.2). Representative domain pairs from each orbit of domain pairs are further analysed in synoptic Table 3.4.3.4 (non-ferroelastic domain pairs) and in synoptic Table 3.4.3.6 (ferroelastic domain pairs).

The set of the twinning groups K_{1j} given in this column is analogous to the concept of a *complete twin* defined as 'an edifice

comprising in addition to an original crystal (domain state \mathbf{S}_1) as many twinned crystals (domain states \mathbf{S}_j) as there are possible twin laws' (see Curien & Le Corre, 1958). If a traditional definition of a twin law ['a geometrical relationship between two crystal components of a twin', see Section 3.3.2 and Koch (2004); Curien & Le Corre (1958)] is applied *sensu stricto* to domain twins then one gets the following correspondence:

(i) a twin law of a non-ferroelastic domain twin is specified by the twinning group K_{1j} (see Section 3.4.3.3 and Table 3.4.3.4);

(ii) two twin laws of two compatible ferroelastic domain twins, resulting from one ferroelastic single-domain pair $\{\mathbf{S}_1, \mathbf{S}_j\}$, are specified by two layer groups \bar{J}_{1j} associated with the twinning group K_{1j} of this ferroelastic single-domain pair $\{(\mathbf{S}_1, \mathbf{S}_j)\}$ (see Section 3.4.3.4 and Table 3.4.3.6).

n : *number of principal single-domain states*, the finest subdivision of domain states in a continuum description, $n = [G : F_1] = |G| : |F_1|$ [see equation (3.4.2.11)].

d_F : *number of principal domain states with the same symmetry group (stabilizer)*, $d_F = [N_G(F_1) : F_1] = |N_G(F_1)| : |F_1|$ [see equation (3.4.2.35)]. If $d_F > 1$, then the group F_1 does not specify the first single-domain state \mathbf{S}_1 . The number n_F of subgroups conjugate with F_1 is $n_F = n : d_F$.

n_e : *number of ferroelectric single-domain states*, $n_e = [G : C_1] = |G| : |C_1|$, where C_1 is the stabilizer (in G) of the spontaneous polarization in the first domain state \mathbf{S}_1 [see equation (3.4.2.32)]. The number d_e of principal domain states compatible with one ferroelectric domain state (degeneracy of ferroelectric domain states) equals $d_e = [C_1 : F_1] = |C_1| : |F_1|$ [see equation (3.4.2.33)].

Aizu's classification of ferroelectric phases (Aizu, 1969; see Table 3.4.2.3): $n_e = n$, fully ferroelectric; $1 < n_e < n$, partially ferroelectric; $n_e = 1$, non-ferroelectric, the parent phase is polar and the spontaneous polarization in the ferroic phase is the same as in the parent phase; $n_e = 0$, non-ferroelectric, parent phase is non-polar.

n_a : *number of ferroelastic single-domain states*, $n_a = [G : A_1] = |G| : |A_1|$, where A_1 is the stabilizer (in G) of the spontaneous strain in the first domain state \mathbf{S}_1 [see equation (3.4.2.28)]. The number d_a of principal domain states compatible with one ferroelastic domain state (degeneracy of ferroelastic domain states) is given by $d_a = [A_1 : F_1] = |A_1| : |F_1|$ [see equation (3.4.2.29)].

Aizu's classification of ferroelastic phases (Aizu, 1969; see Table 3.4.2.3): $n_a = n$, fully ferroelastic; $1 < n_a < n$, partially ferroelastic; $n_e = 1$, non-ferroelastic.

Example 3.4.2.5. Orthorhombic phase of perovskite crystals. The parent phase has symmetry $G = m\bar{3}m$ and the symmetry of the ferroic orthorhombic phase is $F_1 = m_{xy}2_{xy}m_z$. In Table 3.4.2.7, we find that $n = n_e$, i.e. the phase is fully ferroelectric. Then we can associate with each principal domain state a spontaneous polarization. In column K_{1j} there are four twinning groups. As explained in Section 3.4.3, these groups represent four 'twin laws' that can be characterized by the angle between the spontaneous polarization in single-domain state \mathbf{S}_1 and \mathbf{S}_j , $j = 2, 3, 4, 5$. If we choose $\mathbf{P}_{(s)}^{(1)}$ along the direction [110] (F_1 does not specify unambiguously this direction, since $d_F = 2!$), then the angles between $\mathbf{P}_{(s)}^{(1)}$ and $\mathbf{P}_{(s)}^{(j)}$, representing the 'twin law' for these four twinning groups $m\bar{3}m(m_{zx})$, $m\bar{3}m(2_{zx})$, $4_z/m_zm_xm_{xy}$, $m_{xy}m_{xy}^*m_z$, are, respectively, 60, 120, 90 and 180°.

3.4.2.5. Basic (microscopic) domain states and their partition into translation subsets

The examination of principal domain states performed in the continuum approach can be easily generalized to a *microscopic description*. Let us denote the *space-group* symmetry of the parent (high-symmetry) phase by \mathcal{G} and the space group of the

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Table 3.4.2.7. Group-subgroup symmetry descents $G \supset F_1$

G : point-group symmetry of parent phase; F_1 : point-group symmetry of single-domain state S_1 ; Γ_η : representation of G ; $N_G(F_1)$: normalizer of F_1 in G ; $K_G(F_1, g_{ij})$: twinning groups, $g_{ij} \in G$; n : number of principal single-domain states; d_F : number of principal domain states with the same symmetry; n_e : number of ferroelectric single-domain states; n_a : number of ferroelastic single-domain states.

G	F_1	Γ_η	$N_G(F_1)$	$K_G(F_1, g_{ij})$	n	d_F	n_e	n_a
$\bar{1}$	1	A_u	$\bar{1}$	$\bar{1}^*$	2	2	2	1
$2_u \dagger$	1	B	2_u	2_u^*	2	2	2	2
$m_u \dagger$	1	A''	m_u	m_u^*	2	2	2	2
$2_u/m_u \dagger$	m_u	B_u	$2_u/m_u$	$2_u^*/m_u$	2	2	2	1
	2_u	A_u	$2_u/m_u$	$2_u/m_u^*$	2	2	2	1
	$\bar{1}$	B_g	$2_u/m_u$	$2_u^*/m_u^*$	2	2	0	2
	1	Reducible	$2_u/m_u$	$m_u^*, 2_u^*, \bar{1}^*$	4	4	4	2
$2_x 2_y 2_z$	2_z	B_{1g}	$2_x 2_y 2_z$	$2_x^* 2_y^* 2_z^*$	2	2	2	2
	2_x	B_{3g}	$2_x 2_y 2_z$	$2_x^* 2_y^* 2_z^*$	2	2	2	2
	2_y	B_{2g}	$2_x 2_y 2_z$	$2_x^* 2_y^* 2_z^*$	2	2	2	2
	1	Reducible	$2_x 2_y 2_z$	$2_z^*, 2_x^*, 2_y^*$	4	4	4	4
$m_x m_y 2_z$	m_x	B_2	$m_x m_y 2_z$	$m_x m_y^* 2_z^*$	2	2	2	2
	m_y	B_1	$m_x m_y 2_z$	$m_x^* m_y 2_z^*$	2	2	2	2
	2_z	A_2	$m_x m_y 2_z$	$m_x^* m_y^* 2_z^*$	2	2	1	2
	1	Reducible	$m_x m_y 2_z$	$m_x^*, m_y^*, 2_z^*$	4	2	4	4
$m_x m_y m_z$	$m_x m_y 2_z$	B_{1u}	$m_x m_y m_z$	$m_x m_y m_z^*$	2	2	2	1
	$2_x m_y m_z$	B_{3u}	$m_x m_y m_z$	$m_x^* m_y m_z$	2	2	2	1
	$m_x 2_y m_z$	B_{2u}	$m_x m_y m_z$	$m_x m_y^* m_z$	2	2	2	1
	$2_x 2_y 2_z$	A_{1u}	$m_x m_y m_z$	$m_x^* m_y^* m_z^*$	2	2	0	1
	$2_z/m_z$	B_{1g}	$m_x m_y m_z$	$m_x^* m_y^* m_z$	2	2	0	2
	$2_x/m_x$	B_{3g}	$m_x m_y m_z$	$m_x m_y^* m_z^*$	2	2	0	2
	$2_y/m_y$	B_{2g}	$m_x m_y m_z$	$m_x^* m_y m_z^*$	2	2	0	2
	m_z	Reducible	$m_x m_y m_z$	$2_x^* m_y^* m_z, m_x^* 2_y^* m_z, 2_z^*/m_z$	4	4	4	2
	m_x	Reducible	$m_x m_y m_z$	$m_x m_y^* 2_z^*, m_x 2_y^* m_z^*, 2_x^*/m_x$	4	4	4	2
	m_y	Reducible	$m_x m_y m_z$	$m_x^* m_y 2_z^*, 2_x^* m_y m_z^*, 2_y^*/m_y$	4	4	4	2
	2_z	Reducible	$m_x m_y m_z$	$m_x^* m_y^* 2_z, 2_x^* 2_y^* 2_z, 2_z/m_z^*$	4	4	2	2
	2_x	Reducible	$m_x m_y m_z$	$2_x m_y^* m_z^*, 2_x 2_y^* 2_z^*, 2_x/m_x^*$	4	4	2	2
	2_y	Reducible	$m_x m_y m_z$	$m_x^* 2_y m_z^*, 2_x^* 2_y^* 2_z^*, 2_y/m_y^*$	4	4	2	2
	$\bar{1}$	Reducible	$m_x m_y m_z$	$2_z^*/m_z, 2_x^*/m_x, 2_y^*/m_y$	4	4	0	4
1	Reducible	$m_x m_y m_z$	$m_z^*, m_x^*, m_y^*, 2_z^*, 2_x^*, 2_y^*, \bar{1}^*$	8	8	8	4	
4_z	2_z	B	4_z	4_z^*	2	2	1	2
	1	${}^1 E \oplus {}^2 E$	4_z	$4_z, 2_z^*$	4	4	4	4
$\bar{4}_z$	2_z	B	$\bar{4}_z$	$\bar{4}_z^*$	2	2	2	2
	1	${}^1 E \oplus {}^2 E$	$\bar{4}_z$	$\bar{4}_z, 2_z^*$	4	2	4	4
$4_z/m_z$	$\bar{4}_z$	B_u	$4_z/m_z$	$4_z^*/m_z^*$	2	2	0	1
	4_z	A_u	$4_z/m_z$	$4_z/m_z^*$	2	2	2	1
	$2_z/m_z$	B_g	$4_z/m_z$	$4_z^*/m_z$	2	2	0	2
	m_z	${}^1 E_u \oplus {}^2 E_u$	$4_z/m_z$	$4_z/m_z, 2_z^*/m_z$	4	4	4	2
	2_z	Reducible	$4_z/m_z$	$\bar{4}_z^*, 4_z^*, 2_z/m_z^*$	4	4	2	2
	$\bar{1}$	${}^1 E_g \oplus {}^2 E_g$	$4_z/m_z$	$4_z/m_z, 2_z^*/m_z^*$	4	4	0	4
1	Reducible	$4_z/m_z$	$\bar{4}_z, 4_z, m_z^*, 2_z^*, \bar{1}^*$	8	8	8	4	
$4_z 2_x 2_{xy}$	4_z	A_2	$4_z 2_x 2_{xy}$	$4_z 2_x^* 2_{xy}^*$	2	2	2	1
	$2_{xy} 2_{xy} 2_z$	B_2	$4_z 2_x 2_{xy}$	$4_z^* 2_x^* 2_{xy}^*$	2	2	0	2
	$2_x 2_y 2_z$	B_1	$4_z 2_x 2_{xy}$	$4_z^* 2_x^* 2_{xy}^*$	2	2	0	2
	$2_{xy} (2_{x\bar{y}})$	E	$2_{x\bar{y}} 2_{xy} 2_z$	$4_z 2_x^* 2_{xy}^*, 2_{x\bar{y}}^* 2_{xy} 2_z^*$	4	2	2	2
	2_z	Reducible	$4_z 2_x 2_{xy}$	$4_z^*, 2_x^* 2_y^* 2_z^*, 2_{x\bar{y}}^* 2_{xy} 2_z^*$	4	4	2	2
	$2_x (2_y)$	E	$2_{x\bar{y}} 2_{xy} 2_z$	$4_z 2_x^* 2_{xy}^*, 2_x 2_y^* 2_z^*$	4	2	2	2
1	E	$4_z 2_x 2_{xy}$	$4_z, 2_z^*, 2_x^*(2), 2_{xy}^*(2)$	8	8	8	8	
$4_z m_x m_{xy}$	4_z	A_2	$4_z m_x m_{xy}$	$4_z m_x^* m_{xy}^*$	2	2	1	1
	$m_{x\bar{y}} m_{xy} 2_z$	B_2	$4_z m_x m_{xy}$	$4_z^* m_x^* m_{xy}$	2	2	1	2
	$m_x m_y 2_z$	B_1	$4_z m_x m_{xy}$	$4_z^* m_x m_{xy}^*$	2	2	1	2
	$m_{xy} (m_{x\bar{y}})$	E	$m_{x\bar{y}} m_{xy} 2_z$	$4_z m_x m_{xy}, m_{x\bar{y}}^* m_{xy} 2_z^*$	4	2	4	4
	$m_x (m_y)$	E	$m_x m_y 2_z$	$4_z m_x m_{xy}, m_x m_y^* 2_z^*$	4	2	4	4
	2_z	Reducible	$4_z m_x m_{xy}$	$4_z^*, m_x^* m_y^* 2_z, m_{x\bar{y}}^* m_{xy} 2_z^*$	4	4	2	2
	1	E	$4_z m_x m_{xy}$	$4_z, m_x^*(2), m_{xy}^*(2), 2_z^*$	8	8	8	8

$\dagger u = x, y, z, xy, yz, zx, x\bar{y}, y\bar{z}, z\bar{x}, x', x'', y', y''.$

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Table 3.4.2.7 (cont.)

G	F_1	Γ_η	$N_G(F_1)$	$K_G(F_1, g_{1j})$	n	d_F	n_c	n_a	
$\bar{4}_z 2_x m_{xy}$	$\bar{4}_z$	A_2	$\bar{4}_z 2_x m_{xy}$	$\bar{4}_z 2_x^* m_{xy}^*$	2	2	0	1	
	$m_{xy} m_{xy} 2_z$	B_2	$\bar{4}_z 2_x m_{xy}$	$\bar{4}_z 2_x^* m_{xy}^*$	2	2	2	2	
	$2_x 2_y 2_z$	B_1	$\bar{4}_z 2_x m_{xy}$	$\bar{4}_z 2_x^* m_{xy}^*$	2	2	0	2	
	$m_{xy} (m_{xy})$	E	$m_{xy} m_{xy} 2_z$	$\bar{4}_z 2_x m_{xy}, m_{xy}^* m_{xy} 2_z^*$	4	2	4	4	
	2_z	Reducible	$\bar{4}_z 2_x m_{xy}$	$\bar{4}_z^*, m_{xy}^* m_{xy}^* 2_z, 2_x^* 2_y^* 2_z^*$	4	4	2	2	
	$2_x (2_y)$	E	$2_x 2_y 2_z$	$\bar{4}_z 2_x m_{xy}, 2_x 2_y^* 2_z^*$	4	2	4	4	
	1	E	$\bar{4}_z 2_x m_{xy}$	$\bar{4}_z, m_{xy}^*(2), 2_z^*, 2_x^*(2)$	8	8	8	8	
$\bar{4}_z m_x 2_{xy}$	$\bar{4}_z$	A_2	$\bar{4}_z m_x 2_{xy}$	$\bar{4}_z m_x^* 2_{xy}^*$	2	2	0	1	
	$m_x m_y 2_z$	B_2	$\bar{4}_z m_x 2_{xy}$	$\bar{4}_z m_x^* 2_{xy}^*$	2	2	2	2	
	$2_{xy} 2_{xy} 2_z$	B_1	$\bar{4}_z m_x 2_{xy}$	$\bar{4}_z m_x^* 2_{xy}^*$	2	2	0	2	
	$m_x (m_y)$	E	$m_x m_y 2_z$	$\bar{4}_z m_x 2_{xy}, m_x m_y^* 2_z^*$	4	2	4	4	
	$2_{xy} (2_{xy})$	E	$2_{xy} 2_{xy} 2_z$	$\bar{4}_z m_x 2_{xy}, 2_x^* 2_y^* 2_z^*$	4	2	4	4	
	2_z	Reducible	$\bar{4}_z m_x 2_{xy}$	$\bar{4}_z^*, m_x^* m_y^* 2_z, 2_{xy}^* 2_{xy}^* 2_z^*$	4	4	2	2	
	1	E	$\bar{4}_z m_x 2_{xy}$	$\bar{4}_z, m_x^*(2), 2_{xy}^*(2), 2_z^*$	8	8	8	8	
$4_z / m_z m_x m_{xy}$	$\bar{4}_z m_x 2_{xy}$	B_{2u}	$4_z / m_z m_x m_{xy}$	$4_z^* / m_z^* m_x^* m_{xy}^*$	2	2	0	1	
	$\bar{4}_z 2_x m_{xy}$	B_{1u}	$4_z / m_z m_x m_{xy}$	$4_z^* / m_z^* m_x^* m_{xy}^*$	2	2	0	1	
	$4_z m_x m_{xy}$	A_{2u}	$4_z / m_z m_x m_{xy}$	$4_z^* / m_z^* m_x^* m_{xy}^*$	2	2	2	1	
	$\bar{4}_z 2_x 2_{xy}$	A_{1u}	$4_z / m_z m_x m_{xy}$	$4_z^* / m_z^* m_x^* m_{xy}^*$	2	2	0	1	
	$4_z / m_z$	A_{2g}	$4_z / m_z m_x m_{xy}$	$4_z^* / m_z^* m_x^* m_{xy}^*$	2	2	0	1	
	$\bar{4}_z$	Reducible	$4_z / m_z m_x m_{xy}$	$\bar{4}_z 2_x^* m_{xy}^*, 4_z m_x^* 2_{xy}^*, 4_z^* / m_z^*$	4	4	0	1	
	4_z	Reducible	$4_z / m_z m_x m_{xy}$	$4_z m_x^* m_{xy}^*, 4_z^* 2_x^* 2_{xy}^*, 4_z^* / m_z^*$	4	4	2	1	
	$m_{xy} m_{xy} m_z$	B_{2g}	$4_z / m_z m_x m_{xy}$	$4_z^* / m_z^* m_x^* m_{xy}^*$	2	2	0	2	
	$m_x m_y m_z$	B_{1g}	$m_x m_y m_z$	$4_z^* / m_z^* m_x^* m_{xy}^*$	2	2	0	2	
	$2_{xy} m_{xy} m_z (m_{xy} 2_{xy} m_z)$	E_u	$m_{xy} m_{xy} m_z$	$4_z / m_z m_x m_{xy}, m_{xy}^* m_{xy}^* m_z$	4	2	4	2	
	$2_x m_y m_z (m_x 2_y m_z)$	E_u	$m_x m_y m_z$	$4_z / m_z m_x m_{xy}, m_x^* m_y^* m_z$	4	2	4	2	
	$m_{xy} m_{xy} 2_z$	Reducible	$4_z / m_z m_x m_{xy}$	$\bar{4}_z^* 2_x^* m_{xy}^*, 4_z^* m_x^* m_{xy}^*, m_{xy}^* m_{xy}^* m_z^*$	4	4	2	2	
	$m_x m_y 2_z$	Reducible	$4_z / m_z m_x m_{xy}$	$\bar{4}_z^* m_x^* 2_{xy}^*, 4_z^* m_x^* m_{xy}^*, m_x m_y m_z^*$	4	4	2	2	
	$2_{xy} 2_{xy} 2_z$	Reducible	$4_z / m_z m_x m_{xy}$	$\bar{4}_z^* m_x^* 2_{xy}^*, 4_z^* 2_x^* 2_{xy}^*, m_{xy}^* m_{xy}^* m_z^*$	4	4	0	2	
	$2_x 2_y 2_z$	Reducible	$4_z / m_z m_x m_{xy}$	$\bar{4}_z^* 2_x^* m_{xy}^*, 4_z^* 2_x^* 2_{xy}^*, m_x^* m_y^* m_z^*$	4	4	0	2	
	$2_{xy} / m_{xy} (2_{xy} / m_{xy})$	E_g	$m_{xy} m_{xy} m_z$	$4_z / m_z m_x m_{xy}, m_{xy}^* m_{xy}^* m_z$	4	2	0	4	
	$2_z / m_z$	Reducible	$4_z / m_z m_x m_{xy}$	$4_z^* / m_z^*, m_x^* m_y^* m_z^*, m_x^* m_y^* m_z$	4	4	0	4	
	$2_x / m_x (2_y / m_y)$	E_g	$m_x m_y m_z$	$4_z / m_z m_x m_{xy}, m_x m_y m_z^*$	4	2	0	4	
	$m_{xy} (m_{xy})$	Reducible	$m_{xy} m_{xy} m_z$	$\bar{4}_z 2_x m_{xy}, 4_z m_x m_{xy}, 2_{xy}^* m_{xy} m_z^*, m_{xy}^* m_{xy} 2_z^*, 2_{xy}^* / m_{xy}$	8	4	8	4	
	m_z	E_u	$4_z / m_z m_x m_{xy}$	$4_z / m_z, 2_{xy}^* m_x^* m_z^*(2), 2_x^* m_y^* m_z^*(2), 2_z^* / m_z$	8	8	8	4	
	$m_x (m_y)$	Reducible	$m_x m_y m_z$	$\bar{4}_z m_x 2_{xy}, 4_z m_x m_{xy}, m_x m_y^* 2_z^*, m_x 2_y^* m_z^*, 2_x^* / m_x$	8	4	8	4	
	$2_{xy} (2_{xy})$	Reducible	$m_{xy} m_{xy} m_z$	$\bar{4}_z m_x 2_{xy}, 4_z 2_x 2_{xy}, m_{xy}^* 2_{xy} m_z^*, 2_{xy}^* 2_{xy} 2_z^*, 2_{xy} / m_{xy}$	8	4	8	4	
	2_z	Reducible	$4_z / m_z m_x m_{xy}$	$\bar{4}_z^*, 4_z^*, m_x^* m_y^* 2_z, m_{xy}^* m_{xy}^* 2_z, 2_x^* 2_y^* 2_z^*, 2_{xy}^* 2_{xy}^* 2_z^*, 2_z / m_z^*$	8	8	2	4	
	$2_x (2_y)$	Reducible	$m_x m_y m_z$	$\bar{4}_z 2_x m_{xy}, 4_z 2_x 2_{xy}, 2_x m_y^* m_z^*, 2_x 2_y^* 2_z^*, 2_x / m_x$	8	4	4	4	
	$\bar{1}$	E_g	$4_z / m_z m_x m_{xy}$	$4_z / m_z, 2_{xy}^* / m_{xy}^*(2), 2_z^* / m_z^*, 2_x^* / m_x^*(2)$	8	8	0	8	
	1	Reducible	$4_z / m_z m_x m_{xy}$	$\bar{4}_z, 4_z, m_{xy}^*(2), m_x^*, m_y^*(2), 2_{xy}^*(2), 2_z^*, 2_x^*(2), 1^*$	16	16	16	8	
	3_z	1	E	3_z	3_z	3	3	3	3
	$\bar{3}_z$	3_z	A_u	$\bar{3}_z$	$\bar{3}_z^*$	2	2	2	1
$\bar{1}$		E_g	$\bar{3}_z$	$\bar{3}_z$	3	3	0	3	
1		E_u	$\bar{3}_z$	$\bar{3}_z, 3_z, \bar{1}^*$	6	6	6	3	
$3_z 2_x$	3_z	A_2	$3_z 2_x$	$3_z 2_x^*$	2	2	2	1	
	$2_x (2_x', 2_x'')$	E	2_x	$3_z 2_x$	3	1	3	3	
	1	E	$3_z 2_x$	$3_z, 2_x^*(3)$	6	6	6	6	
$3_z 2_y$	3_z	A_2	$3_z 2_y$	$3_z 2_y^*$	2	2	2	1	
	$2_y (2_y', 2_y'')$	E	2_y	$3_z 2_y$	3	1	3	3	
	1	E	$3_z 2_y$	$3_z, 2_y^*(3)$	6	6	6	6	
$3_z m_x$	3_z	A_2	$3_z m_x$	$3_z m_x^*$	2	2	1	1	
	$m_x (m_x', m_x'')$	E	m_x	$3_z m_x$	3	1	3	3	
	1	E	$3_z m_x$	$3_z, m_x^*(3)$	6	6	6	6	
$3_z m_y$	3_z	A_2	$3_z m_y$	$3_z m_y^*$	2	2	1	1	
	$m_y (m_y', m_y'')$	E	m_y	$3_z m_y$	3	1	3	3	
	1	E	$3_z m_y$	$3_z, m_y^*(3)$	6	6	6	6	

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

Table 3.4.2.7 (cont.)

G	F_1	Γ_η	$N_G(F_1)$	$K_G(F_1, g_{1j})$	n	d_F	n_c	n_a
$\bar{3}_z m_x$	$3_z m_x$	A_{2u}	$\bar{3}_z m_x$	$\bar{3}_z^* m_x$	2	2	2	1
	$3_z 2_x$	A_{1u}	$\bar{3}_z m_x$	$\bar{3}_z^* m_x^*$	2	2	0	1
	$\bar{3}_z$	A_{2g}	$\bar{3}_z m_x$	$\bar{3}_z^* m_x^*$	2	2	0	1
	3_z	Reducible	$\bar{3}_z m_x$	$3_z m_x^*, 3_z 2_x^*, \bar{3}_z^*$	4	4	2	1
	$2_x/m_x (2_{x'}/m_{x'}, 2_{x''}/m_{x''})$	E_g	$2_x/m_x$	$\bar{3}_z m_x$	3	1	0	3
	$m_x (m_{x'}, m_{x''})$	E_u	$2_x/m_x$	$\bar{3}_z m_x, 3_z m_x, 2_x^*/m_x(3)$	6	2	6	3
	$2_x (2_{x'}, 2_{x''})$	E_u	$2_x/m_x$	$\bar{3}_z m_x, 3_z 2_x, 2_x/m_x^*(3)$	6	2	6	3
	$\bar{1}$	E_g	$\bar{3}_z m_x$	$\bar{3}_z, 2_x^*/m_x^*(3)$	6	6	0	6
	1	E_u	$\bar{3}_z m_x$	$\bar{3}_z, 3_z, m_x^*(3), 2_x^*(3), \bar{1}^*$	12	12	12	6
	$\bar{3}_z m_y$	$3_z m_y$	A_{2u}	$\bar{3}_z m_y$	$\bar{3}_z^* m_y$	2	2	2
$3_z 2_y$		A_{1u}	$\bar{3}_z m_y$	$\bar{3}_z^* m_y^*$	2	2	0	1
$\bar{3}_z$		A_{2g}	$\bar{3}_z m_y$	$\bar{3}_z^* m_y^*$	2	2	0	1
3_z		Reducible	$\bar{3}_z m_y$	$3_z m_y^*, 3_z 2_y^*, \bar{3}_z^*$	4	4	0	1
$2_y/m_y (2_{y'}/m_{y'}, 2_{y''}/m_{y''})$		E_g	$2_y/m_y$	$\bar{3}_z m_y$	3	1	2	1
$m_y (m_{y'}, m_{y''})$		E_u	$2_y/m_y$	$\bar{3}_z m_y, 3_z m_y, 2_y^*/m_y(3)$	6	2	0	3
$2_y (2_{y'}, 2_{y''})$		E_u	$2_y/m_y$	$\bar{3}_z m_y, 3_z 2_y, 2_y/m_y^*(3)$	6	2	6	3
$\bar{1}$		E_g	$\bar{3}_z m_y$	$\bar{3}_z, 2_y^*/m_y^*(3)$	6	6	0	3
1		E_u	$\bar{3}_z m_y$	$\bar{3}_z, 3_z, m_y^*(3), 2_y^*(3), \bar{1}^*$	12	12	12	6
6_z		3_z	B	6_z	6_z^*	2	2	1
	2_z	E_2	6_z	6_z	3	3	1	3
	1	E_1	6_z	$6_z, 3_z, 2_z^*$	6	6	6	6
$\bar{6}_z$	3_z	A''	$\bar{6}_z$	$\bar{6}_z^*$	2	2	2	1
	m_z	E'	$\bar{6}_z$	$\bar{6}_z$	3	2	3	3
	1	E''	$\bar{6}_z$	$\bar{6}_z, 3_z, m_z^*$	6	6	6	6
$6_z/m_z$	$\bar{6}_z$	B_u	$6_z/m_z$	$6_z^*/m_z$	2	2	0	1
	6_z	A_u	$6_z/m_z$	$6_z/m_z^*$	2	2	2	1
	$\bar{3}_z$	B_g	$6_z/m_z$	$6_z^*/m_z^*$	2	2	0	1
	3_z	Reducible	$6_z/m_z$	$6_z^*, 6_z, \bar{3}_z^*$	4	4	2	1
	$2_z/m_z$	E_{2g}	$6_z/m_z$	$6_z/m_z$	3	3	0	3
	m_z	E_{1u}	$6_z/m_z$	$6_z/m_z, \bar{6}_z, 2_z^*/m_z$	6	6	6	3
	2_z	E_{2u}	$6_z/m_z$	$6_z/m_z, 6_z, 2_z/m_z^*$	6	6	2	3
	$\bar{1}$	E_{1g}	$6_z/m_z$	$6_z/m_z, \bar{3}_z, 2_z^*/m_z^*$	6	6	0	6
	1	Reducible	$6_z/m_z$	$\bar{6}_z, 6_z, \bar{3}_z, 3_z, m_z^*, 2_z^*, \bar{1}^*$	12	12	12	6
	$6_z 2_x 2_y$	6_z	A_2	$6_z 2_x 2_y$	$6_z 2_x^* 2_y^*$	2	2	2
$3_z 2_x$		B_1	$6_z 2_x 2_y$	$6_z^* 2_x^* 2_y^*$	2	2	0	1
$3_z 2_y$		B_2	$6_z 2_x 2_y$	$6_z^* 2_x^* 2_y$	2	2	0	1
3_z		Reducible	$6_z 2_x 2_y$	$6_z^*, 3_z 2_x^*, 3_z 2_y^*$	4	4	2	1
$2_x 2_y 2_z (2_{x'} 2_{y'} 2_z, 2_{x''} 2_{y''} 2_z)$		E_2	$2_x 2_y 2_z$	$6_z 2_x 2_y$	3	1	0	3
2_z		E_2	$6_z 2_x 2_y$	$6_z, 2_x^* 2_y^* 2_z(3)$	6	6	2	6
$2_x (2_{x'}, 2_{x''})$		E_1	$2_x 2_y 2_z$	$6_z 2_x 2_y, 3_z 2_x, 2_x 2_y^* 2_z^*$	6	2	6	6
$2_y (2_{y'}, 2_{y''})$		E_1	$2_x 2_y 2_z$	$6_z 2_x 2_y, 3_z 2_y, 2_x^* 2_y^* 2_z^*$	6	2	6	6
1		E_1	$6_z 2_x 2_y$	$6_z, 3_z, 2_z^*, 2_x^*(3), 2_y^*(3)$	12	12	12	12
$6_z m_x m_y$		6_z	A_2	$6_z m_x m_y$	$6_z m_x^* m_y^*$	2	2	1
	$3_z m_x$	B_2	$6_z m_x m_y$	$6_z^* m_x^* m_y^*$	2	2	1	1
	$3_z m_y$	B_1	$6_z m_x m_y$	$6_z^* m_x^* m_y$	2	2	1	1
	3_z	Reducible	$6_z m_x m_y$	$6_z^*, 3_z m_x^*, 3_z m_y^*$	4	4	1	1
	$m_x m_y 2_z (m_{x'} m_{y'} 2_z, m_{x''} m_{y''} 2_z)$	E_2	$m_x m_y 2_z$	$6_z m_x m_y$	3	1	1	3
	$m_x (m_{x'}, m_{x''})$	E_1	$m_x m_y 2_z$	$6_z m_x m_y, 3_z m_x, m_x m_y^* 2_z^*$	6	2	6	6
	$m_y (m_{y'}, m_{y''})$	E_1	$m_x m_y 2_z$	$6_z m_x m_y, 3_z m_y, m_x^* m_y^* 2_z^*$	6	2	6	6
	2_z	E_2	$6_z m_x m_y$	$6_z, m_x^* m_y^* 2_z(3)$	6	6	1	6
	1	E_1	$6_z m_x m_y$	$6_z, 3_z, 2_z^*, m_x^*(3), m_y^*(3)$	12	12	12	12
	$\bar{6}_z m_x 2_y$	$\bar{6}_z$	A_2'	$\bar{6}_z m_x 2_y$	$\bar{6}_z m_x^* 2_y^*$	2	2	0
$3_z m_x$		A_2''	$\bar{6}_z m_x 2_y$	$\bar{6}_z^* m_x^* 2_y^*$	2	2	2	1
$3_z 2_y$		A_1'	$\bar{6}_z m_x 2_y$	$\bar{6}_z^* m_x^* 2_y$	2	2	0	1
3_z		Reducible	$\bar{6}_z m_x 2_y$	$\bar{6}_z^*, 3_z m_x^*, 3_z 2_y^*$	4	4	2	1
$m_x 2_y 2_z (m_{x'} 2_{y'} 2_z, m_{x''} 2_{y''} 2_z)$		E'	$m_x 2_y 2_z$	$\bar{6}_z m_x 2_y$	3	1	3	3
m_z		E'	$\bar{6}_z m_x 2_y$	$\bar{6}_z, m_x^* 2_y^* 2_z(3)$	6	6	6	6
$m_x (m_{x'}, m_{x''})$		E''	$m_x 2_y 2_z$	$\bar{6}_z m_x 2_y, 3_z m_x, m_x 2_y^* 2_z^*$	6	2	6	6
$2_y (2_{y'}, 2_{y''})$		E''	$m_x 2_y 2_z$	$\bar{6}_z m_x 2_y, 3_z 2_y, m_x^* 2_y^* 2_z^*$	6	2	3	6
1		E''	$\bar{6}_z m_x 2_y$	$\bar{6}_z, 3_z, m_x^*, m_x^*(3), 2_y^*(3)$	12	12	12	12

3.4. DOMAIN STRUCTURES

Table 3.4.2.7 (cont.)

G	F_1	Γ_η	$N_G(F_1)$	$K_G(F_1, g_{1j})$	n	d_F	n_c	n_a	
$\bar{6}_2 2_x m_y$	$\bar{6}_z$	A_2'	$\bar{6}_z 2_x m_y$	$\bar{6}_z 2_x^* m_y^*$	2	2	0	1	
	$3_z m_y$	A_2'	$\bar{6}_z 2_x m_y$	$\bar{6}_z 2_x^* m_y$	2	2	2	1	
	$3_z 2_x$	A_1''	$\bar{6}_z 2_x m_y$	$\bar{6}_z 2_x^* m_y^*$	2	2	0	1	
	3_z	Reducible	$\bar{6}_z 2_x m_y$	$\bar{6}_z^*, 3_z m_y^*, 3_z 2_x^*$	4	4	2	1	
	$2_x m_y m_z (2_x m_y m_z, 2_{x'} m_{y'} m_z)$	E'	$m_x 2_y m_z$	$\bar{6}_z 2_x m_y$	3	1	3	3	
	m_z	E'	$\bar{6}_z 2_x m_y$	$\bar{6}_z, 2_x^* m_y^* m_z(3)$	6	6	6	6	
	$m_y (m_{y'}, m_{y''})$	E''	$m_x 2_y m_z$	$\bar{6}_z 2_x m_y, 3_z m_y, 2_x^* m_y m_z^*$	6	2	6	6	
	$2_x (2_{x'}, 2_{x''})$	E''	$m_x 2_y m_z$	$\bar{6}_z 2_x m_y, 3_z 2_x, 2_x m_y^* m_z^*$	6	2	3	6	
	1	E''	$\bar{6}_z 2_x m_y$	$\bar{6}_z, 3_z, m_x^*, m_y^*(3), 2_x^*(3)$	12	12	12	12	
	$6_z/m_z m_x m_y$	$\bar{6}_z m_x 2_y$	B_{2u}	$6_z/m_z m_x m_y$	$6_z^*/m_z m_x m_y^*$	2	2	0	1
$\bar{6}_z 2_x m_y$		B_{1u}	$6_z/m_z m_x m_y$	$6_z^*/m_z m_x^* m_y$	2	2	0	1	
$6_z m_x m_y$		A_{2u}	$6_z/m_z m_x m_y$	$6_z/m_z^* m_x m_y$	2	2	2	1	
$6_z 2_x 2_y$		A_{1u}	$6_z/m_z m_x m_y$	$6_z/m_z^* m_x^* m_y^*$	2	2	0	1	
$6_z/m_z$		A_{2g}	$6_z/m_z m_x m_y$	$6_z/m_z m_x^* m_y^*$	2	2	0	1	
$\bar{6}_z$		Reducible	$6_z/m_z m_x m_y$	$\bar{6}_z m_x^* 2_y^*, \bar{6}_z 2_x^* m_y^*, 6_z^*/m_z$	4	4	0	1	
6_z		Reducible	$6_z/m_z m_x m_y$	$6_z m_x^* m_y^*, 6_z 2_x^* 2_y^*, 6_z/m_z^*$	4	4	2	1	
$\bar{3}_z m_x$		B_{1g}	$6_z/m_z m_x m_y$	$6_z^*/m_z^* m_x m_y^*$	2	2	0	1	
$\bar{3}_z m_y$		B_{2g}	$6_z/m_z m_x m_y$	$6_z^*/m_z^* m_x^* m_y$	2	2	0	1	
$3_z m_x$		Reducible	$6_z/m_z m_x m_y$	$\bar{6}_z^* m_x 2_y^*, 6_z^* m_x m_y^*, \bar{3}_z^* m_x$	4	4	2	1	
$3_z m_y$		Reducible	$6_z/m_z m_x m_y$	$\bar{6}_z^* 2_x^* m_y, 6_z^* m_x^* m_y, \bar{3}_z^* m_y$	4	4	2	1	
$3_z 2_x$		Reducible	$6_z/m_z m_x m_y$	$\bar{6}_z^* 2_x m_y^*, 6_z^* 2_x 2_y^*, \bar{3}_z^* m_x^*$	4	4	0	1	
$3_z 2_y$		Reducible	$6_z/m_z m_x m_y$	$\bar{6}_z^* m_x^* 2_y, 6_z^* 2_x 2_y, \bar{3}_z^* m_y^*$	4	4	0	1	
$\bar{3}_z$		Reducible	$6_z/m_z m_x m_y$	$6_z^*/m_z^*, \bar{3}_z m_x^*, \bar{3}_z m_y^*$	4	4	0	1	
3_z		Reducible	$6_z/m_z m_x m_y$	$\bar{6}_z^*, 6_z^*, 3_z m_x^*, 3_z m_y^*, 3_z 2_x^*, 3_z 2_y^*, \bar{3}_z^*$	8	8	2	1	
$m_x m_y m_z (m_{x'} m_{y'} m_z, m_{x''} m_{y''} m_z)$		E_{2g}	$m_x m_y m_z$	$6_z/m_z m_x m_y$	3	1	0	3	
$m_x m_y 2_z (m_{x'} m_{y'} 2_z, m_{x''} m_{y''} 2_z)$		E_{2u}	$m_x m_y m_z$	$6_z/m_z m_x m_y, 6_z m_x m_y, m_x m_y m_z^*$	6	2	2	3	
$2_x m_y m_z (2_{x'} m_{y'} m_z, 2_{x''} m_{y''} m_z)$		E_{1u}	$m_x m_y m_z$	$6_z/m_z m_x m_y, \bar{6}_z 2_x m_y, m_x^* m_y m_z$	6	2	6	3	
$m_x 2_y m_z (m_{x'} 2_{y'} m_z, m_{x''} 2_{y''} m_z)$		E_{1u}	$m_x m_y m_z$	$6_z/m_z m_x m_y, \bar{6}_z m_x 2_y, m_x m_y^* m_z$	6	2	6	3	
$2_x 2_y 2_z (2_{x'} 2_{y'} 2_z, 2_{x''} 2_{y''} 2_z)$		E_{2u}	$m_x m_y m_z$	$6_z/m_z m_x m_y, 6_z 2_x 2_y, m_x^* m_y^* m_z^*$	6	6	0	3	
$2_z/m_z$		E_{2g}	$6_z/m_z m_x m_y$	$6_z/m_z, m_x^* m_y^* m_z(3)$	6	6	0	6	
$2_x/m_x (2_{x'}/m_{x'}, 2_{x''}/m_{x''})$		E_{1g}	$m_x m_y m_z$	$6_z/m_z m_x m_y, \bar{3}_z m_x, m_x m_y^* m_z^*$	6	2	0	6	
$2_y/m_y (2_{y'}/m_{y'}, 2_{y''}/m_{y''})$		E_{1g}	$m_x m_y m_z$	$6_z/m_z m_x m_y, \bar{3}_z m_y, m_x^* m_y m_z^*$	6	2	0	6	
m_z		E_{1u}	$6_z/m_z m_x m_y$	$6_z/m_z, \bar{6}_z, 2_x^* m_y^* m_z, m_x^* 2_y^* m_z, 2_z^*/m_z$	12	12	12	6	
$m_x (m_{x'}, m_{x''})$		Reducible	$m_x m_y m_z$	$\bar{6}_z m_x 2_y, 6_z m_x m_y, \bar{3}_z m_x, 3_z m_x, m_x m_y^* 2_z^*, m_x 2_y^* m_z^*, 2_x^*/m_x$	12	4	12	6	
$m_y (m_{y'}, m_{y''})$		Reducible	$m_x m_y m_z$	$\bar{6}_z 2_x m_y, 6_z m_x m_y, \bar{3}_z m_y, 3_z m_y, m_x^* m_y 2_z^*, 2_x^* m_y^* m_z^*, 2_y^*/m_y$	12	4	12	6	
2_z		E_{2u}	$6_z/m_z m_x m_y$	$6_z/m_z, 6_z, m_x^* m_y^* 2_z(3), 2_x^* 2_y^* 2_z(3), 2_z/m_z^*$	12	12	2	6	
$2_x (2_{x'}, 2_{x''})$		Reducible	$m_x m_y m_z$	$\bar{6}_z 2_x m_y, 6_z 2_x 2_y, \bar{3}_z m_x, 3_z 2_x, 2_x m_y^* m_z^*, 2_x 2_y^* 2_z, 2_x/m_x^*$	12	4	6	6	
$2_y (2_{y'}, 2_{y''})$		Reducible	$m_x m_y m_z$	$\bar{6}_z m_x 2_y, 6_z 2_x 2_y, \bar{3}_z m_y, 3_z 2_y, m_x^* 2_y m_z^*, 2_x^* 2_y^* 2_z, 2_y/m_y^*$	12	4	6	6	
$\bar{1}$		E_{1g}	$6_z/m_z m_x m_y$	$6_z/m_z, \bar{3}_z, 2_z^*/m_z^*, 2_x^*/m_x^*(3), 2_y^*/m_y^*(3)$	12	12	0	12	
1		Reducible	$6_z/m_z m_x m_y$	$\bar{6}_z, 6_z, \bar{3}_z, 3_z, m_x^*, m_x^*(3), m_y^*(3), 2_z^*, 2_x^*(3), 2_y^*(3), \bar{1}^*$	24	24	24	12	
23		$3_p (3_q, 3_r, 3_s)$	T	3_p	23	4	1	4	4
		$2_x 2_y 2_z$	E	23	23	3	3	0	3
		$2_z (2_x, 2_y)$	T	$2_x 2_y 2_z$	$23, 2_x^* 2_y^* 2_z$	6	2	6	6
		1	T	23	$3_p(4), 2_x^*(3)$	12	12	12	12
$m\bar{3}$		23	A_u	$m\bar{3}$	$m^* \bar{3}^*$	2	2	0	1
		$\bar{3}_p (\bar{3}_q, \bar{3}_r, \bar{3}_s)$	T_g	$\bar{3}_p$	$m\bar{3}$	4	1	0	4
	$3_p (3_q, 3_r, 3_s)$	T_u	$\bar{3}_p$	$m\bar{3}, 23$	8	2	8	4	
	$m_x m_y m_z$	E_g	$m\bar{3}$	$m\bar{3}$	3	3	0	3	
	$m_x m_y 2_z (2_x m_y m_z, m_x 2_y m_z)$	T_u	$m_x m_y m_z$	$m\bar{3}, m_x m_y m_z^*$	6	2	6	3	
	$2_x 2_y 2_z$	E_u	$m\bar{3}$	$m\bar{3}, 23, m_x^* m_y^* m_z^*$	6	6	0	3	
	$2_z/m_z (2_x/m_x, 2_y/m_y)$	T_g	$m_x m_y m_z$	$m\bar{3}, m_x^* m_y^* m_z$	6	2	0	6	
	$m_z (m_x, m_y)$	T_u	$m_x m_y m_z$	$m\bar{3}, 2_x^* m_y^* m_z, m_x^* 2_y^* m_z, 2_z^*/m_z$	12	4	12	6	
	$2_z (2_x, 2_y)$	Reducible	$m_x m_y m_z$	$m\bar{3}, 23, m_x^* m_y^* 2_z, 2_x^* 2_y^* 2_z, 2_z/m_z^*$	12	4	6	6	
	$\bar{1}$	T_g	$m\bar{3}$	$\bar{3}_p(4), 2_z^*/m_z^*(3)$	12	12	0	12	
	1	T_u	$m\bar{3}$	$\bar{3}_p(4), 3_p(4), m_x^*(3), 2_x^*(3), \bar{1}^*$	24	24	24	12	

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

Table 3.4.2.7 (cont.)

G	F_1	Γ_η	$N_G(F_1)$	$K_G(F_1, g_{1j})$	n	d_F	n_c	n_a
432	23	A_2	432	4^*32^*	2	2	0	1
	$3_p 2_{x\bar{y}} (3_q 2_{x\bar{y}}, 3_r 2_{xy}, 3_s 2_{xy})$	T_2	$3_p 2_{x\bar{y}}$	432	4	1	0	4
	$3_p (3_q, 3_r, 3_s)$	T_1	$3_p 2_{x\bar{y}}$	$23, 3_p 2_{x\bar{y}}^*$	8	2	8	4
	$4_z 2_x 2_{xy} (4_x 2_y 2_{yz}, 4_y 2_z 2_{xz})$	E	$4_z 2_x 2_{xy}$	432	3	1	0	3
	$4_z (4_x, 4_y)$	T_1	$4_z 2_x 2_{xy}$	$432, 4_z 2_x 2_{xy}^*$	6	2	6	3
	$2_x 2_y 2_z$	E	432	$23, 4_z^* 2_x 2_{xy}^*$	6	6	0	6
	$2_{xy} 2_{xy} 2_z (2_{yz} 2_{yz} 2_x, 2_{zx} 2_{zx} 2_y)$	T_2	$4_z 2_x 2_{xy}$	$432, 4_z^* 2_x 2_{xy}^*$	6	2	0	6
	$2_z (2_x, 2_y)$	Reducible	$4_z 2_x 2_{xy}$	$23, 4_y 2_z 2_{xy}, 4_z^*, 2_x^* 2_y^* 2_z^*, 2_x^* 2_y^* 2_z^*$	12	4	6	12
	$2_{xy} (2_{yz}, 2_{zx}, 2_{x\bar{y}}, 2_{y\bar{z}}, 2_{z\bar{x}})$	T_1, T_2	$2_{x\bar{y}} 2_{xy} 2_z$	$432, 3_r 2_{xy}, 3_s 2_{xy}, 4_z 2_x 2_{xy}, 2_{x\bar{y}} 2_{xy} 2_z^*$	12	2	12	12
	1	T_1, T_2	432	$3_p(4), 4_z(3), 2_z^*(3), 2_{xy}^*(6)$	24	24	24	24
	$\bar{4}3m$	23	A_2	$\bar{4}3m$	$\bar{4}^*3m^*$	2	2	0
$3_p m_{x\bar{y}} (3_q m_{x\bar{y}}, 3_r m_{xy}, 3_s m_{xy})$		T_2	$3_p m_{x\bar{y}}$	$\bar{4}3m$	4	1	4	4
$3_p (3_q, 3_r, 3_s)$		T_1	$3_p m_{x\bar{y}}$	$\bar{4}3m, 23, 3_p m_{x\bar{y}}^*$	8	2	4	4
$\bar{4}_z 2_x m_{xy} (\bar{4}_x 2_y m_{yz}, \bar{4}_y 2_z m_{zx})$		E	$\bar{4}_z 2_x m_{xy}$	$\bar{4}3m$	3	1	0	3
$\bar{4}_z (\bar{4}_x, \bar{4}_y)$		T_1	$\bar{4}_z 2_x m_{xy}$	$\bar{4}3m, \bar{4}_z 2_x m_{xy}^*$	6	2	0	3
$m_{x\bar{y}} m_{xy} 2_z (m_{yz} m_{yz} 2_x, m_{zx} m_{zx} 2_y)$		T_2	$\bar{4}_z 2_x m_{xy}$	$\bar{4}3m, \bar{4}_z^* 2_x m_{xy}^*$	6	2	6	6
$2_x 2_y 2_z$		E	$\bar{4}3m$	$23, \bar{4}_z^* 2_x m_{xy}^*$	6	6	0	6
$m_{xy} (m_{yz}, m_{zx}, m_{x\bar{y}}, m_{y\bar{z}}, m_{z\bar{x}})$		T_1, T_2	$m_{x\bar{y}} m_{xy} 2_z$	$\bar{4}3m, 3, m_{xy}, 3, m_{xy}, \bar{4}_z 2_x m_{xy}, m_{x\bar{y}}^* m_{xy} 2_z^*$	12	2	12	12
$2_z (2_x, 2_y)$		Reducible	$\bar{4}_z 2_x m_{xy}$	$23, \bar{4}_z^*, 4_z^*, m_{x\bar{y}}^* m_{xy}^* 2_z^*, 2_x^* 2_y^* 2_z^*$	12	4	6	12
1		T_1, T_2	$\bar{4}3m$	$3_p(4), \bar{4}_z(3), m_{xy}^*(6), 2_z^*(3)$	24	24	24	24
$m\bar{3}m$		$\bar{4}3m$	A_{2u}	$m\bar{3}m$	$m^* \bar{3}^* m$	2	2	0
	432	A_{1u}	$m\bar{3}m$	$m^* \bar{3}^* m^*$	2	2	0	1
	$m\bar{3}$	A_{2g}	$m\bar{3}m$	$m\bar{3}m^*$	2	2	0	1
	23	Reducible	$m\bar{3}m$	$\bar{4}^* 3m^*, 4^* 32^*, m_z^* \bar{3}_p$	4	4	0	1
	$\bar{3}_p m_{x\bar{y}} (\bar{3}_q m_{x\bar{y}}, \bar{3}_r m_{xy}, \bar{3}_s m_{xy})$	T_{2g}	$\bar{3}_p m_{x\bar{y}}$	$m\bar{3}m$	4	1	0	4
	$3_p m_{x\bar{y}} (3_q m_{x\bar{y}}, 3_r m_{xy}, 3_s m_{xy})$	T_{1u}	$\bar{3}_p m_{x\bar{y}}$	$m\bar{3}m, \bar{4}3m, \bar{3}_p^* m_{x\bar{y}}$	8	2	8	4
	$3_p 2_{x\bar{y}} (3_q 2_{x\bar{y}}, 3_r 2_{xy}, 3_s 2_{xy})$	T_{2u}	$\bar{3}_p m_{x\bar{y}}$	$m\bar{3}m, 432, \bar{3}_p^* m_{x\bar{y}}$	8	2	0	4
	$\bar{3}_p (\bar{3}_q, \bar{3}_r, \bar{3}_s)$	T_{1g}	$\bar{3}_p m_{x\bar{y}}$	$m\bar{3}m, m\bar{3}, \bar{3}_p^* m_{x\bar{y}}$	8	2	0	4
	$3_p (3_q, 3_r, 3_s)$	Reducible	$\bar{3}_p m_{x\bar{y}}$	$\bar{4}3m, 432, m\bar{3}, 23, 3_p m_{x\bar{y}}^*, 3_p 2_{x\bar{y}}^*, \bar{3}_p^*$	16	4	8	4
	$4_z / m_x m_x m_{xy} (4_x / m_x m_x m_{yz}, 4_y / m_y m_y m_{zx})$	E_g	$4_z / m_z m_x m_{xy}$	$m\bar{3}m$	3	1	0	3
	$\bar{4}_z 2_x m_{xy} (\bar{4}_x 2_y m_{yz}, \bar{4}_y 2_z m_{zx})$	E_u	$4_z / m_z m_x m_{xy}$	$m\bar{3}m, \bar{4}3m, 4_z^* / m_z^* m_x^* m_{xy}^*$	6	2	0	3
	$\bar{4}_z m_x m_{xy} (\bar{4}_x m_y m_{yz}, \bar{4}_y m_z m_{zx})$	T_{2u}	$4_z / m_z m_x m_{xy}$	$m\bar{3}m, 4_z^* / m_z^* m_x^* m_{xy}^*$	6	2	0	3
	$4_z m_x m_{xy} (4_x m_y m_{yz}, 4_y m_z m_{zx})$	T_{1u}	$4_z / m_z m_x m_{xy}$	$m\bar{3}m, 4_z / m_z^* m_x^* m_{xy}^*$	6	2	6	3
	$4_z 2_x 2_{xy} (4_x 2_y 2_{yz}, 4_y 2_z 2_{xz})$	E_u	$4_z / m_z m_x m_{xy}$	$m\bar{3}m, 432, 4_z / m_z^* m_x^* m_{xy}^*$	6	2	0	3
	$4_z / m_z (4_x / m_x, 4_y / m_y)$	T_{1g}	$4_z / m_z m_x m_{xy}$	$m\bar{3}m, 4_z / m_z^* m_x^* m_{xy}^*$	6	2	0	3
	$\bar{4}_z (\bar{4}_x, \bar{4}_y)$	Reducible	$4_z / m_z m_x m_{xy}$	$m\bar{3}m, \bar{4}3m, \bar{4}_z 2_x m_{xy}^*, \bar{4}_z m_x^* 2_{xy}^*, 4_z^* / m_z^*$	12	4	0	3
	$4_z (4_x, 4_y)$	Reducible	$4_z / m_z m_x m_{xy}$	$m\bar{3}m, 432, 4_z m_x^* m_{xy}^*, 4_z 2_x^* 2_{xy}^*, 4_z / m_z^*$	12	4	6	3
	$m_x m_y m_z$	E_g	$m\bar{3}m$	$m\bar{3}, 4_z^* / m_z^* m_x^* m_{xy}^*$	6	6	0	6
	$m_{x\bar{y}} m_{xy} m_z (m_{yz} m_{yz} m_x, m_{zx} m_{zx} m_y)$	T_{2g}	$4_z / m_z m_x m_{xy}$	$m\bar{3}m, 4_z^* / m_z^* m_x^* m_{xy}^*$	6	2	0	6
	$m_x m_y 2_z (2_x m_y m_z, m_x 2_y m_z)$	Reducible	$4_z / m_z m_x m_{xy}$	$m\bar{3}, 4_y / m_y m_y m_{zx}, \bar{4}_z^* m_x^* 2_{xy}^*, 4_z^* m_x^* m_{xy}^*$	12	4	6	6
	$m_{x\bar{y}} m_{xy} 2_z (m_{yz} m_{yz} 2_x, m_{zx} m_{zx} 2_y)$	Reducible	$4_z / m_z m_x m_{xy}$	$m\bar{3}m, \bar{4}3m, \bar{4}_z^* 2_x^* m_{xy}^*, 4_z^* m_x^* m_{xy}^*, m_{x\bar{y}}^* m_{xy}^* m_z^*$	12	4	6	6
	$m_{x\bar{y}} 2_{xy} m_z (m_{yz} 2_{yz} m_x, m_{zx} 2_{zx} m_y, 2_{x\bar{y}} m_{xy} m_z, 2_{y\bar{z}} m_{yz} m_x, 2_{z\bar{x}} m_{zx} m_y)$	T_{1u}, T_{2u}	$m_{x\bar{y}} m_{xy} m_z$	$m\bar{3}m(m_{zx}), m\bar{3}m(2_{zx}), 4_z / m_z m_x m_{xy}, m_{x\bar{y}}^* m_{xy}^* m_z^*$	12	2	12	6
	$2_x 2_y 2_z$	E_u	$m\bar{3}m$	$m\bar{3}, 23, \bar{4}_z^* 2_x^* m_{xy}^*, 4_z^* 2_x^* 2_{xy}^*, m_x^* m_y^* m_z^*$	12	12	0	6
	$2_{xy} 2_{xy} 2_z (2_{yz} 2_{yz} 2_x, 2_{zx} 2_{zx} 2_y)$	Reducible	$4_z / m_z m_x m_{xy}$	$m\bar{3}m, 432, \bar{4}_z m_x^* 2_{xy}^*, 4_z^* 2_x^* 2_{xy}^*, m_{x\bar{y}}^* m_{xy}^* m_z^*$	12	4	0	6
	$2_z / m_z (2_x / m_x, 2_y / m_y)$	Reducible	$4_z / m_z m_x m_{xy}$	$m\bar{3}, 4_y / m_y m_y m_{zx}, 4_z^* / m_z^*, m_x^* m_y^* m_z^*$	12	4	0	12
	$2_{xy} / m_{xy} (2_{yz} / m_{yz}, 2_{zx} / m_{zx}, 2_{x\bar{y}} / m_{x\bar{y}}, 2_{y\bar{z}} / m_{y\bar{z}}, 2_{z\bar{x}} / m_{z\bar{x}})$	T_{1g}, T_{2g}	$m_{x\bar{y}} m_{xy} m_z$	$m\bar{3}m, \bar{3}_p m_{xy}^* m_z^*$	12	2	0	12
	$m_z (m_x, m_y)$	T_{1u}, T_{2u}	$4_z / m_z m_x m_{xy}$	$m\bar{3}, \bar{4}_z m_x 2_{yz}, 4_y m_y m_{zx}, 4_z / m_z, 2_x^* m_y^* m_z^*(2), m_{x\bar{y}}^* 2_{xy}^* m_z^*(2), 2_z^* / m_z^*$	24	8	24	12
	$m_{xy} (m_{yz}, m_{zx}, m_{x\bar{y}}, m_{y\bar{z}}, m_{z\bar{x}})$	T_{1u}	$m_{x\bar{y}} m_{xy} m_z$	$m\bar{3}m, \bar{4}3m, 4_z 2_x m_{xy}, 4_z m_x m_{xy}, \bar{3}_p m_{xy}, \bar{3}_s m_{xy}, 3_s m_{xy}, m_{x\bar{y}}^* m_{xy}^* 2_z^*, 2_{xy}^* / m_{xy}^*$	24	4	24	12
	$2_z (2_x, 2_y)$	Reducible	$4_z / m_z m_x m_{xy}$	$m\bar{3}, 23, 4_z 2_x m_{zx}, 4_y 2_z m_{zx}, 4_z^*, 4_z^* m_x^* m_y^* 2_z^*, m_{x\bar{y}}^* m_{xy}^* 2_z^*$	24	8	6	12
	$2_{xy} (2_{yz}, 2_{zx}, 2_{x\bar{y}}, 2_{y\bar{z}}, 2_{z\bar{x}})$	T_{2u}	$m_{x\bar{y}} m_{xy} m_z$	$m\bar{3}m, 432, 3, m_{xy}, 3, m_{xy}, 3, 2_{xy}, 3, 2_{xy}, 4_z m_x 2_{xy}, 4_z 2_x 2_{xy}, m_{x\bar{y}}^* 2_{xy}^* m_z^*, 2_{xy}^* 2_{xy}^* 2_z^*, 2_{xy} / m_{xy}^*$	24	4	12	12
	$\bar{1}$	T_{1g}, T_{2g}	$m\bar{3}m$	$\bar{3}_p(4), 4_z / m_z(3), 2_z^* / m_z^*(3), 2_{xy}^* / m_{xy}^*(6)$	24	24	0	24
	1	T_{1u}, T_{2u}	$m\bar{3}m$	$\bar{3}_p(4), \bar{4}_z(3), 4_z(3), m_z^*(3), m_{xy}^*(6), 2_z^*(3), 2_{xy}^*(6), 1^*$	48	48	48	24

3.4. DOMAIN STRUCTURES

ferroic (low-symmetry) phase by \mathcal{F}_1 , which is a proper subgroup of \mathcal{G} , $\mathcal{F}_1 \subset \mathcal{G}$. Further we denote by \mathcal{S}_1 a *basic (microscopic)* low-symmetry structure described by positions of atoms in the unit cell. The stabilizer $\mathcal{I}_{\mathcal{G}}(\mathcal{S}_1)$ of the basic structure \mathcal{S}_1 in a single-domain orientation is equal to the space group \mathcal{F}_1 of the ferroic (low-symmetry) phase,

$$\mathcal{I}_{\mathcal{G}}(\mathcal{S}_1) = \mathcal{F}_1. \quad (3.4.2.41)$$

By applying a lost symmetry operation g_j on \mathcal{S}_1 , one gets a crystallographically equivalent low-symmetry basic structure \mathcal{S}_j ,

$$g_j \mathcal{S}_1 = \mathcal{S}_j \neq \mathcal{S}_1, \quad g_j \in \mathcal{G}, \quad g_j \notin \mathcal{F}_1. \quad (3.4.2.42)$$

We may recall that g_j is a space-group symmetry operation consisting of a rotation (point-group operation) g_j and a non-primitive translation $\mathbf{u}(g_j)$, $g_j = \{g_j | \mathbf{u}(g_j)\}$ (see Section 1.2.3). The symbol $\{g_j | \mathbf{u}(g_j)\}$ is called a *Seitz space-group symbol* (Bradley & Cracknell, 1972). The product (composition law) of two Seitz symbols is

$$\{g_1 | \mathbf{u}(g_1)\} \{g_2 | \mathbf{u}(g_2)\} = \{g_1 g_2 | g_1 \mathbf{u}(g_2) + \mathbf{u}(g_1)\}. \quad (3.4.2.43)$$

All crystallographically equivalent low-symmetry basic structures form a \mathcal{G} -orbit and can be calculated from the first basic structure \mathcal{S}_1 in the following way:

$$\mathcal{G}\mathcal{S}_1 = \{\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_j, \dots, \mathcal{S}_N\} = \{e\mathcal{S}_1, g_2\mathcal{S}_1, \dots, g_j\mathcal{S}_1, \dots, g_N\mathcal{S}_1\}, \quad (3.4.2.44)$$

where $g_1 = e$, $g_2, \dots, g_j, \dots, g_N$ are the representatives of the left cosets $g_j \mathcal{F}_1$ of the decomposition of \mathcal{G} ,

$$\mathcal{G} = \mathcal{F}_1 \cup g_2 \mathcal{F}_1 \cup \dots \cup g_j \mathcal{F}_1 \cup \dots \cup g_N \mathcal{F}_1. \quad (3.4.2.45)$$

These crystallographically equivalent low-symmetry structures are called *basic (elementary) domain states*.

The number N of basic domain states is equal to the number of left cosets in the decomposition (3.4.2.45). As we shall see in next section, this number is finite [see equation (3.4.2.60)], though the groups \mathcal{G} and \mathcal{F}_1 consist of an infinite number of operations.

In a microscopic description, a *basic (elementary) domain state* is described by positions of atoms in the unit cell. Basic domain states that are related by translations suppressed at the phase transition are called *translational* or *antiphase domain states*. These domain states have the same macroscopic properties. The attribute 'to have the same macroscopic properties' divides all basic domain states into classes of translational domain states.

In a microscopic description, a ferroic phase transition is accompanied by a lowering of space-group symmetry from a parent space group \mathcal{G} , with translation subgroup \mathcal{T} and point group G , to a low-symmetry space group \mathcal{F}_1 , with translation subgroup \mathcal{U}_1 and point group F_1 . There exists a unique intermediate group \mathcal{M}_1 , called the *Hermann group*, which has translation subgroup \mathcal{T} and point group $M_1 = F_1$ (see e.g. Hahn & Wondratschek, 1994; Wadhawan, 2000; Wondratschek & Aroyo, 2001):

$$\mathcal{F}_1 \stackrel{c}{\subset} \mathcal{M}_1 \stackrel{t}{\subset} \mathcal{G}, \quad (3.4.2.46)$$

$$F_1 = M_1 \subseteq G, \quad (3.4.2.47)$$

$$\mathcal{U}_1 \subseteq \mathcal{T} = \mathcal{T}, \quad (3.4.2.48)$$

where $\stackrel{c}{\subset}$ denotes an equiclass subgroup (a descent at which only the translational subgroup is reduced but the point group is preserved) and $\stackrel{t}{\subset}$ signifies an equitranslational subgroup (only the point group descends but the translational subgroup does not change). Group \mathcal{M}_1 is a maximal subgroup of \mathcal{G} that preserves all macroscopic properties of the basic domain state \mathcal{S}_1 with symmetry \mathcal{F}_1 .

At this point we have to make an important note. Any space-group symmetry descent $\mathcal{G} \subset \mathcal{F}_1$ requires that the lengths of the basis vectors of the translation group \mathcal{U}_1 of the ferroic space group \mathcal{F}_1 are commensurate with basic vectors of the translational group \mathcal{T} of the parent space group \mathcal{G} . It is usually tacitly assumed that this condition is fulfilled, although in real phase transitions this is never the case. Lattice parameters depend on temperature and are, therefore, different in parent and ferroic phases. At ferroelastic phase transitions the spontaneous strain changes the lengths of the basis vectors in different ways and at first-order phase transitions the lattice parameters change abruptly.

To assure the validity of translational symmetry descents, we have to suppress all distortions of the crystal lattice. This condition, called the *high-symmetry approximation* (Zikmund, 1984) or *parent clamping approximation* (PCA) (Janovec *et al.*, 1989; Wadhawan, 2000), requires that the lengths of the basis vectors $\mathbf{a}^f \mathbf{b}^f \mathbf{c}^f$ of the translation group \mathcal{U}_1 of the ferroic space group \mathcal{F}_1 are either exactly the same as, or are integer multiples of, the basic vectors $\mathbf{a}^p \mathbf{b}^p \mathbf{c}^p$ of the translational group \mathcal{T} of the parent space group \mathcal{G} . Then the relation between the primitive basis vectors $\mathbf{a}^f \mathbf{b}^f \mathbf{c}^f$ of \mathcal{U}_1 and the primitive basis vectors $\mathbf{a}^p \mathbf{b}^p \mathbf{c}^p$ of \mathcal{T} can be expressed as

$$(\mathbf{a}^f, \mathbf{b}^f, \mathbf{c}^f) = (\mathbf{a}^p, \mathbf{b}^p, \mathbf{c}^p) \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix}, \quad (3.4.2.49)$$

where m_{ij} , $i, j = 1, 2, 3$, are integers.

Throughout this part, the parent clamping approximation is assumed to be fulfilled.

Now we can return to the partition of the set of basic domain states into translational subsets. Let $\{\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_d\}$ be the set of all basic translational domain states that can be generated from \mathcal{S}_1 by lost translations. The stabilizer (in \mathcal{G}) of this set is the Hermann group,

$$\mathcal{I}_{\mathcal{G}}\{\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_d\} = \mathcal{M}_1, \quad (3.4.2.50)$$

which plays the role of the intermediate group. The number of translational subsets and the relation between these subsets is determined by the decomposition of \mathcal{G} into left cosets of \mathcal{M}_1 :

$$\mathcal{G} = \{g_1 | \mathbf{v}(g_1)\} \mathcal{M}_1 \cup \{g_2 | \mathbf{v}(g_2)\} \mathcal{M}_1 \cup \dots \cup \{g_j | \mathbf{v}(g_j)\} \mathcal{M}_1 \cup \dots \cup \{g_n | \mathbf{v}(g_n)\} \mathcal{M}_1. \quad (3.4.2.51)$$

Representatives $g_j = \{g_j | \mathbf{u}(g_j)\}$ are space-group operations, where g_j is a point-group operation and $\mathbf{u}(g_j)$ is a non-primitive translation (see Section 1.2.3).

We note that the Hermann group \mathcal{M}_1 can be found in the software *GI★KoBo-1* as the equitranslational subgroup of \mathcal{G} with the point-group descent $G \subset F_1$ for any space group \mathcal{G} and any point group F_1 of the ferroic phase.

The decomposition of the point group G into left cosets of the point group F_1 is given by equation (3.4.2.10):

$$G = g_1 F_1 \cup g_2 F_1 \cup \dots \cup g_j F_1 \cup \dots \cup g_n F_1. \quad (3.4.2.52)$$

Since the space groups \mathcal{M}_1 and \mathcal{F}_1 have identical point groups, $M_1 = F_1$, the decomposition (3.4.2.51) is identical with a decomposition of G into left cosets of M_1 ; one can, therefore, choose for the representatives in (3.4.2.10) the point-group parts of the representatives $\{g_j | \mathbf{u}(g_j)\}$ in decomposition (3.4.2.51). Both decompositions comprise the same number of left cosets, *i.e.* corresponding indices are equal; therefore, the number of subsets, comprising only translational basic domain states, is equal to the number n of principal domain states:

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

$$n = [\mathcal{G} : \mathcal{M}_1] = [G : F_1] = |G| : |F_1|, \quad (3.4.2.53)$$

where $|G|$ and $|F_1|$ are the number of operations of G and F_1 , respectively.

The first ‘representative’ basic domain state S_j of each subset can be obtained from the first basic domain state S_1 :

$$S_j = \{g_j | \mathbf{v}(g_j)\} S_1, \quad j = 1, 2, \dots, n, \quad (3.4.2.54)$$

where $\{g_j | \mathbf{v}(g_j)\}$ are representatives of left cosets of \mathcal{M}_1 in the decomposition (3.4.2.51).

Now we determine basic domain states belonging to the first subset (first principal domain state). Equiclass groups \mathcal{M}_1 and \mathcal{F}_1 have the same point-group operations and differ only in translations. The decomposition of \mathcal{M}_1 into left cosets of \mathcal{F}_1 can therefore be written in the form

$$\mathcal{M}_1 = \{e | \mathbf{t}_1\} \mathcal{F}_1 \cup \{e | \mathbf{t}_2\} \mathcal{F}_1 \cup \dots \cup \{e | \mathbf{t}_k\} \mathcal{F}_1 \cup \dots \cup \{e | \mathbf{t}_{d_t}\} \mathcal{F}_1, \quad (3.4.2.55)$$

where e is the identity point-group operation and \mathcal{T}_k , $k = 1, 2, \dots, d_t$, are lost translations that can be identified with the representatives in the decomposition of \mathcal{T} into left cosets of \mathcal{U}_1 :

$$\mathcal{T} = \mathbf{t}_1 \mathcal{U}_1 + \mathbf{t}_2 \mathcal{U}_1 + \dots + \mathbf{t}_k \mathcal{U}_1 + \dots + \mathbf{t}_{d_t} \mathcal{U}_1. \quad (3.4.2.56)$$

The number d_t of basic domain states belonging to one principal domain state will be called a *translational degeneracy*. For the translations $\mathbf{t}_1, \mathbf{t}_2, \dots, \mathbf{t}_k, \dots, \mathbf{t}_{d_t}$, one can choose vectors that lead from the origin of a ‘superlattice’ primitive unit cell of \mathcal{U}_1 to lattice points of \mathcal{T} located within or on the side faces of this ‘superlattice’ primitive unit cell. The number d_t of such lattice points is equal to the ratio $v_{\mathcal{F}} : v_{\mathcal{G}}$, where $v_{\mathcal{F}}$ and $v_{\mathcal{G}}$ are the volumes of the *primitive* unit cells of the low-symmetry and parent phases, respectively.

The number d_t can be also expressed as the determinant $\det(m_{ij})$ of the (3×3) matrix of the coefficients m_{ij} that in equation (3.4.2.49) relate the primitive basis vectors $\mathbf{a}^f, \mathbf{b}^f, \mathbf{c}^f$ of \mathcal{U}_1 to the primitive basis vectors $\mathbf{a}^p, \mathbf{b}^p, \mathbf{c}^p$ of \mathcal{T} (Van Tendeloo & Amelincx, 1974; see also Example 2.5 in Section 3.2.3.3). Finally, the number d_t equals the ratio $Z_{\mathcal{F}} : Z_{\mathcal{G}}$, where $Z_{\mathcal{F}}$ and $Z_{\mathcal{G}}$ are the numbers of chemical formula units in the *primitive* unit cell of the ferroic and parent phases, respectively. Thus we get for the translational degeneracy d_t three expressions:

$$d_t = [\mathcal{M}_1 : \mathcal{F}_1] = [\mathcal{T} : \mathcal{U}] = v_{\mathcal{F}} : v_{\mathcal{G}} = \det(m_{ij}) = Z_{\mathcal{F}} : Z_{\mathcal{G}}. \quad (3.4.2.57)$$

The basic domain states belonging to the first subset of translational domain states are

$$S_j = \{e | \mathbf{t}_k\} S_1, \quad k = 1, 2, \dots, d_t, \quad (3.4.2.58)$$

where $\{e | \mathbf{t}_k\}$ is a representative from the decomposition (3.4.2.55).

The partitioning we have just described provides a useful labelling of basic domain states: Any basic domain state can be given a label ab , where the first integer $a = 1, 2, \dots, n$ specifies the principal domain state (translational subset) and the integer $b = 1, 2, \dots, d_t$ designates the domain state within a subset. With this convention the k th basic domain state in the j th subset can be obtained from the first basic domain state $S_1 = S_{11}$ (see Proposition 3.2.3.30 in Section 3.2.3.3):

$$S_{jk} = \{g_j | \mathbf{v}(g_j)\} \{e | \mathbf{t}_k\} S_{11}, \quad j = 1, 2, \dots, n, \quad k = 1, 2, \dots, d_t. \quad (3.4.2.59)$$

In a shorthand version, the letter S can be omitted and the symbol can be written in the form a_b , where the ‘large’ number a signifies the principal domain state and the subscript b (transla-

tional index) specifies a basic domain state compatible with the principal domain state a .

The number n of translational subsets (which can be associated with principal domain states) times the translational degeneracy d_t (number of translational domain states within one translational subset) is equal to the total number N of all basic domain states:

$$\begin{aligned} N &= nd_t = (|G| : |F_1|)(v_{\mathcal{F}} : v_{\mathcal{G}}) = (|G| : |F_1|) \det(m_{ij}) \\ &= (|G| : |F_1|)(Z_{\mathcal{F}} : Z_{\mathcal{G}}). \end{aligned} \quad (3.4.2.60)$$

Example 3.4.2.6. Basic domain states in gadolinium molybdate (GMO). Gadolinium molybdate $[\text{Gd}_2(\text{MoO}_4)_3]$ undergoes a non-equitranslational ferroic phase transition with parent space group $\mathcal{G} = P4_2m (D_{2d}^3)$ and with ferroic space group $\mathcal{F}_1 = Pba2 (C_{2v}^8)$ (see Section 3.1.2). From equation (3.4.2.53) we get $n = |42m| : |mm2| = 8 : 4 = 2$, i.e. there are two subsets of translational domain states corresponding to two principal domain states. In the software *GI★KoBo-1* one finds for the space group $P4_2m$ and the point group $mm2$ the corresponding equitranslational subgroup $\mathcal{M}_1 = Cmm2 (C_{2v}^{11})$ with vectors of the conventional orthorhombic unit cell (in the parent clamping approximation) $\mathbf{a}^o = \mathbf{a}^t - \mathbf{b}^t, \mathbf{b}^o = \mathbf{a}^t + \mathbf{b}^t, \mathbf{c}^o = \mathbf{c}^t$, where $\mathbf{a}^t, \mathbf{b}^t, \mathbf{c}^t$ is the basis of the tetragonal space group $P4_2m$. Hence, according to equation (3.4.2.49),

$$(\mathbf{a}^o, \mathbf{b}^o, \mathbf{c}^o) = (\mathbf{a}^t, \mathbf{b}^t, \mathbf{c}^t) \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (3.4.2.61)$$

The determinant of the transformation matrix equals two, therefore, according to equation (3.4.2.57), each principal domain state can contain $d_t = 2$ translational domain states that are related by lost translation \mathbf{a}^t or \mathbf{b}^t . In all, there are four basic domain states (for more details see Barkley & Jeitschko, 1973; Janovec, 1976; Wondratschek & Jeitschko, 1976).

Example 3.4.2.7. Basic domain states in calomel crystals. Crystals of calomel, Hg_2Cl_2 , consist of almost linear Cl—Hg—Cl molecules aligned parallel to the c axis. The centres of gravity of these molecules form in the parent phase a tetragonal body-centred parent phase with the conventional tetragonal basis $\mathbf{a}^t, \mathbf{b}^t, \mathbf{c}^t$ and with space group $\mathcal{G} = I4/mmm$. The structure of this phase projected onto the $z = 0$ plane is depicted in the middle of Fig. 3.4.2.5 as a solid square with four full circles and one empty circle representing the centres of gravity of the Hg_2Cl_2 molecules at the levels $z = 0$ and $z = c/2$, respectively.

The ferroic phase has point-group symmetry $F_1 = m_{xy}m_{x\bar{y}}2_z$, hence there are $n = |42m| : |m_{xy}m_{x\bar{y}}2_z| = 2$ ferroelastic principal domain states. The conventional orthorhombic basis is $\mathbf{a}^o = \mathbf{a}^t - \mathbf{b}^t, \mathbf{b}^o = \mathbf{a}^t + \mathbf{b}^t, \mathbf{c}^o = \mathbf{c}^t$ (see upper left corner of Fig. 3.4.2.5). This is the same situation as in the previous example, therefore, according to equations (3.4.2.57) and (3.4.2.61), the translational degeneracy $d_t = 2$, i.e. each ferroelastic domain state can contain two basic domain states.

The structure S_1 of the ferroic phase in the parent clamping approximation is depicted in the left-hand part of Fig. 3.4.2.5 with a dotted orthorhombic conventional unit cell. The arrows represent exaggerated spontaneous shifts of the molecules. These shifts are frozen-in displacements of a transverse acoustic soft mode with the \mathbf{k} vector along the $[110]$ direction in the first domain state S_1 , hence all molecules in the (110) plane passing through the origin O are shifted along the $[110]$ direction, whereas those in the neighbouring parallel planes are shifted along the antiparallel direction $[1\bar{1}0]$ (the indices are related to the tetragonal coordinate system). The symmetry of S_1 is described by the space group $\mathcal{F}_1 = Amam (D_{2h}^{17})$; this symbol is related to the conventional orthorhombic basis and the origin of

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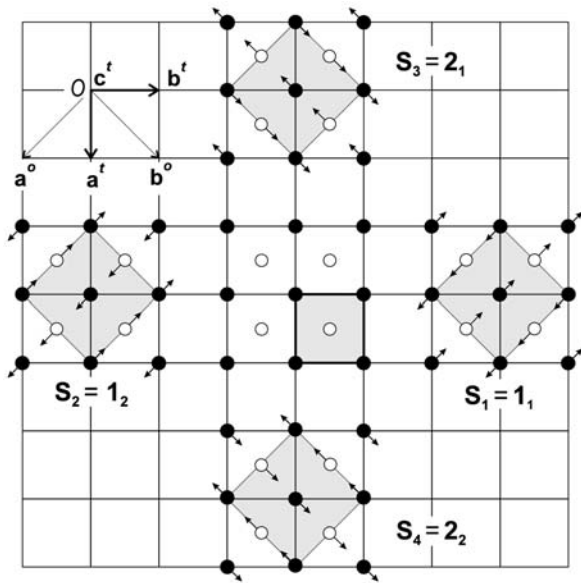


Fig. 3.4.2.5. Four basic single-domain states $S_1 = 1_1$, $S_2 = 1_2$, $S_3 = 2_1$, $S_4 = 2_2$ of the ferroic phase of a calomel (Hg_2Cl_2) crystal. Full \bullet and empty \circ circles represent centres of gravity of Hg_2Cl_2 molecules at the levels $z = 0$ and $z = c/2$, respectively, projected onto the $z = 0$ plane. The parent tetragonal phase is depicted in the centre of the figure with a full square representing the primitive unit cell. Arrows are exaggerated spontaneous shifts of molecules in the ferroic phase. Dotted squares depict conventional unit cells of the orthorhombic basic domain states in the parent clamping approximation. If the parent clamping approximation is lifted, these unit cells would be represented by rectangles elongated parallel to the arrows.

this group is shifted by $\mathbf{a}'/2$ or \mathbf{b} with respect to the origin 0 of the group $\mathcal{G} = I4/mmm$.

Three more basic domain states S_2 , S_3 and S_4 can be obtained, according to equation (3.4.2.44), from S_1 by applying representatives of the left cosets in the resolution of \mathcal{G} [see equation (3.4.2.42)], for which one can find the expression

$$\mathcal{G} = \{1|000\}\mathcal{F}_1 \cup \{1|100\}\mathcal{F}_1 \cup \{4_z|000\}\mathcal{F}_1 \cup \{4_z^3|000\}\mathcal{F}_1. \quad (3.4.2.62)$$

All basic domain states S_1 , S_2 , S_3 and S_4 are depicted in Fig. 3.4.2.5. Domain states S_1 and S_2 , and similarly S_3 and S_4 , are related by lost translation \mathbf{a}' or \mathbf{b}' . Thus the four basic domain states S_1 , S_2 , S_3 and S_4 can be partitioned into two translational subsets $\{S_1, S_2\}$ and $\{S_3, S_4\}$. Basic domain states forming one subset have the same value of the secondary macroscopic order parameter λ , which is in this case the difference $\varepsilon_{11} - \varepsilon_{22}$ of the components of a symmetric second-rank tensor ε , e.g. the permittivity or the spontaneous strain (which is zero in the parent clamping approximation).

This partition provides a useful labelling of basic domain states: $S_1 = 1_1$, $S_2 = 1_2$, $S_3 = 2_1$, $S_4 = 2_2$, where the first number signifies the ferroic (orientational) domain state and the subscript (translational index) specifies the basic domain state with the same ferroic domain state.

Symmetry groups (stabilizers in \mathcal{G}) of basic domain states can be calculated from a space-group version of equation (3.4.2.13):

$$\begin{aligned} \mathcal{F}_2 &= \{1|100\}\mathcal{F}_1\{1|100\}^{-1} = \mathcal{F}_1; \\ \mathcal{F}_3 &= \{4_z|000\}\mathcal{F}_1\{4_z|000\}^{-1} = Bbmm, \end{aligned}$$

with the same conventional basis, and $\mathcal{F}_4 = \{1|100\}\mathcal{F}_3\{1|100\}^{-1} = \mathcal{F}_3$, where the origin of these groups is shifted by $\mathbf{a}'/2$ or \mathbf{b} with respect to the origin 0 of the group $\mathcal{G} = I4/mmm$.

In general, a space-group-symmetry descent $\mathcal{G} \supset \mathcal{F}_1$ can be performed in two steps:

(1) An equitranslational symmetry descent $\mathcal{G} \supseteq \mathcal{M}_1$, where \mathcal{M}_1 is the equitranslational subgroup of \mathcal{G} (Hermann group), which is unequivocally specified by space group \mathcal{G} and by the point group F_1 of the space group \mathcal{F}_1 . The Hermann group \mathcal{M}_1 can be found in the software *GI★KoBo-1* or, in some cases, in *IT A* (2005) under the entry ‘Maximal non-isomorphic subgroups, type I’.

(2) An equiclass symmetry descent $\mathcal{M}_1 \supseteq \mathcal{F}_1$, which can be of three kinds [for more details see *IT A* (2005), Section 2.2.15]:

(i) Space groups \mathcal{M}_1 and \mathcal{F}_1 have the same conventional unit cell. These descents occur only in space groups \mathcal{M}_1 with centred conventional unit cells and the lost translations are some or all centring translations of the unit cell of \mathcal{M}_1 . In many cases, the descent $\mathcal{M}_1 \supseteq \mathcal{F}_1$ can be found in the main tables of *IT A* (2005), under the entry ‘Maximal non-isomorphic subgroups, type IIa’. Gadolinium molybdate belongs to this category.

(ii) The conventional unit cell of \mathcal{M}_1 is larger than that of \mathcal{F}_1 . Some vectors of the conventional unit cell of \mathcal{U}_1 are multiples of that of \mathcal{T} . In many cases, the descent $\mathcal{M}_1 \supseteq \mathcal{F}_1$ can be found in the main tables of *IT A* (2005), under the entry ‘Maximal non-isomorphic subgroups, type IIb’.

(iii) Space group \mathcal{F}_1 is an isomorphic subgroup of \mathcal{M}_1 , i.e. both groups are of the same space-group type (with the same Hermann–Mauguin symbol) or of the enantiomorphic space-group type. Each space group has an infinite number of isomorphic subgroups. Maximal isomorphic subgroups of lowest index are tabulated in *IT A* (2005), under the entry ‘Maximal non-isomorphic subgroups, type IIc’.

3.4.3. Domain pairs: domain twin laws, distinction of domain states and switching

Different domains observed by a single apparatus can exhibit different properties even though their crystal structures are either the same or enantiomorphic and differ only in spatial orientation. Domains are usually distinguished by their bulk properties, i.e. according to their domain states. Then the problem of domain distinction is reduced to the distinction of domain states. To solve this task, we have to describe in a convenient way the distinction of any two of all possible domain states. For this purpose, we use the concept of domain pair.

Domain pairs allow one to express the geometrical relationship between two domain states (the ‘twin law’), determine the distinction of two domain states and define switching fields that may induce a change of one state into the other. Domain pairs also present the first step in examining domain twins and domain walls.

In this section, we define domain pairs, ascribe to them symmetry groups and so-called twinning groups, and give a classification of domain pairs. Then we divide domain pairs into equivalence classes (G -orbits of domain pairs) – which comprise domain pairs with the same inherent properties but with different orientations and/or locations in space – and examine the relation between G -orbits and twinning groups.

A qualitative difference between the coexistence of two domain states provides a basic division into non-ferroelastic and ferroelastic domain pairs. The synoptic Table 3.4.3.4 lists representatives of all G -orbits of *non-ferroelastic domain pairs*, contains information about the distinction of non-ferroelastic domain states by means of diffraction techniques and specifies whether or not important property tensors can distinguish between domain states of a non-ferroelastic domain pair. These data also determine the external fields needed to switch the first domain state into the second domain state of a domain pair. Synoptic Table 3.4.3.6 contains representative *ferroelastic domain pairs* of G -orbits of domain pairs for which there exist compatible (permissible) domain walls and gives for each representative pair the orientation of the *two compatible domain walls*, the expres-