3. PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

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 $[1\bar{1}0]$ direction, whereas those in the neighbouring parallel planes are shifted along the antiparallel direction $[\bar{1}10]$ (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 this group is shifted by $\mathbf{a}^t/2$ 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

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

$$(3.4.2.62)$$

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 $\mathbf{a}^t$ or $\mathbf{b}^t$. 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: $S_1 \equiv 1_1$, $S_2 \equiv 1_2$, $S_3 \equiv 2_1$, $S_1 \equiv 2_2$, 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):

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

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 $\mathbf{a}^t/2$ 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 $\mathcal{G} \overset{t}{\supseteq} \mathcal{M}_1$, 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 (2002) under the entry 'Maximal non-isomorphic subgroups, type I'.

(2) An equiclass symmetry descent $\mathcal{M}_1 \overset{c}{\supseteq} \mathcal{F}_1$, which can be of three kinds [for more details see *IT* A (2002), 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 (2002),

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 (2002), 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 (2002), 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 expression for the disorientation angle (obliquity) and other data. Table 3.4.3.7 lists representatives of all classes of ferroelastic domain pairs for which *no compatible domain walls* exist. Since Table 3.4.2.7 contains for each symmetry descent $G \supset F$ all twinning groups that specify different G-orbits of domain pairs which can appear in the ferroic phase, one can get from this table and from Tables 3.4.3.4, 3.4.3.6 and 3.4.3.7 the significant features of the domain structure of any ferroic phase.

3.4.3.1. *Domain pairs and their symmetry, twin law*

A pair of two domain states, in short a *domain pair*, consists of two domain states, say S_i and S_k, that are considered irrespective of their possible coexistence (Janovec, 1972). Geometrically,

domain pairs can be visualized as two interpenetrating structures of $\mathbf{S}_i$ and $\mathbf{S}_k$. Algebraically, two domain states $\mathbf{S}_i$ and $\mathbf{S}_k$ can be treated in two ways: as an ordered or an unordered pair (see Section 3.2.3.1.2).

An *ordered domain pair*, denoted $(\mathbf{S}_i, \mathbf{S}_k)$, consists of the first domain state $\mathbf{S}_i$ and the second domain state. Occasionally, it is convenient to consider a *trivial ordered domain pair* $(\mathbf{S}_i, \mathbf{S}_i)$ composed of two identical domain states $\mathbf{S}_i$.

An ordered domain pair is a construct that in bicrystallography is called a *dichromatic complex* (see Section 3.3.3; Pond & Vlachavas, 1983; Sutton & Balluffi, 1995; Wadhawan, 2000).

An ordered domain pair $(\mathbf{S}_i, \mathbf{S}_k)$ is defined by specifying $\mathbf{S}_i$ and $\mathbf{S}_k$ or by giving $\mathbf{S}_i$ and a *switching operation* g_{ik} that transforms $\mathbf{S}_i$ into $\mathbf{S}_k$,

$$\mathbf{S}_k = g_{ik}\mathbf{S}_i, \quad \mathbf{S}_i, \mathbf{S}_k \in G\mathbf{S}_1, \quad g_{ik} \in G. \qquad (3.4.3.1)$$

For a given $\mathbf{S}_i$ and $\mathbf{S}_k$, the switching operation g_{ik} is not uniquely defined since each operation from the left coset $g_{ik}F_i$ [where F_i is the stabilizer (symmetry group) of $\mathbf{S}_i$] transforms $\mathbf{S}_i$ into $\mathbf{S}_k$, $g_{ik}\mathbf{S}_i = (g_{ik}F_i)\mathbf{S}_i = \mathbf{S}_k$.

An ordered domain pair $(\mathbf{S}_k, \mathbf{S}_i)$ with a reversed order of domain states is called a *transposed domain pair* and is denoted $(\mathbf{S}_i, \mathbf{S}_k)^t \equiv (\mathbf{S}_k, \mathbf{S}_i)$. A non-trivial ordered domain pair $(\mathbf{S}_i, \mathbf{S}_k)$ is different from the transposed ordered domain pair,

$$(\mathbf{S}_k, \mathbf{S}_i) \neq (\mathbf{S}_i, \mathbf{S}_k) \quad \text{for} \quad i \neq k. \qquad (3.4.3.2)$$

If g_{ik} is a switching operation of an ordered domain pair $(\mathbf{S}_i, \mathbf{S}_k)$, then the inverse operation g_{ik}^{-1} of g_{ik} is a switching operation of the transposed domain pair $(\mathbf{S}_k, \mathbf{S}_i)$:

$$\text{if } (\mathbf{S}_i, \mathbf{S}_k) = (\mathbf{S}_i, g_{ik}\mathbf{S}_i) \text{ and } (\mathbf{S}_k, \mathbf{S}_i) = (\mathbf{S}_k, g_{ki}\mathbf{S}_k), \text{ then } g_{ki} = g_{ik}^{-1}.$$
$$(3.4.3.3)$$

An *unordered domain pair*, denoted by $\{\mathbf{S}_i, \mathbf{S}_k\}$, is defined as an *unordered* set consisting of two domain states $\mathbf{S}_i$ and $\mathbf{S}_k$. In this case, the sequence of domains states in a domain pair is irrelevant, therefore

$$\{\mathbf{S}_i, \mathbf{S}_k\} = \{\mathbf{S}_k, \mathbf{S}_i\}. \qquad (3.4.3.4)$$

In what follows, we shall omit the specification 'ordered' or 'unordered' if it is evident from the context, or if it is not significant.

A domain pair $(\mathbf{S}_i, \mathbf{S}_k)$ can be transformed by an operation $g \in G$ into another domain pair,

$$g(\mathbf{S}_i, \mathbf{S}_k) \equiv (g\mathbf{S}_i, g\mathbf{S}_k) = (\mathbf{S}_l, \mathbf{S}_m), \quad \mathbf{S}_i, \mathbf{S}_k, \mathbf{S}_l, \mathbf{S}_m \in G\mathbf{S}_1, \quad g \in G.$$
$$(3.4.3.5)$$

These two domain pairs will be called *crystallographically equivalent (in G) domain pairs* and will be denoted $(\mathbf{S}_i, \mathbf{S}_k) \overset{G}{\sim} (\mathbf{S}_l, \mathbf{S}_m)$.

If the transformed domain pair is a transposed domain pair $(\mathbf{S}_k, \mathbf{S}_i)$, then the operation g will be called a *transposing operation*,

$$g^\star(\mathbf{S}_i, \mathbf{S}_k) = (g^\star\mathbf{S}_i, g^\star\mathbf{S}_k) = (\mathbf{S}_k, \mathbf{S}_i), \quad \mathbf{S}_i, \mathbf{S}_k \in G\mathbf{S}_1, \quad g^\star \in G.$$
$$(3.4.3.6)$$

We see that a transposing operation $g^\star \in G$ exchanges domain states $\mathbf{S}_i$ and $\mathbf{S}_k$:

$$g^\star\mathbf{S}_i = \mathbf{S}_k, \quad g^\star\mathbf{S}_k = \mathbf{S}_i, \quad \mathbf{S}_i, \mathbf{S}_k \in G\mathbf{S}_1, \quad g^\star \in G. \qquad (3.4.3.7)$$

Thus, comparing equations (3.4.3.1) and (3.4.3.7), we see that a transposing operation $g^\star$ is a switching operation that transforms $\mathbf{S}_i$ into $\mathbf{S}_k$, and, in addition, switches $\mathbf{S}_k$ into $\mathbf{S}_i$. Then a product of two transposing operations is an operation that changes neither $\mathbf{S}_i$ nor $\mathbf{S}_k$.

What we call in this chapter a *transposing operation* is usually denoted as a *twin operation* (see Section 3.3.5 and *e.g.* Holser, 1958*a*; Curien & Donnay, 1959; Koch, 1999). We are reserving the term 'twin operation' for operations that exchange domain states of a simple domain twin in which two ferroelastic domain states *coexist* along a domain wall. Then, as we shall see, the transposing operations are identical with the twin operations in non-ferroelastic domains (see Section 3.4.3.5) but may differ in ferroelastic domain twins, where only some transposing operations of a single-domain pair survive as twin operations of the corresponding ferroelastic twin with a nonzero disorientation angle (see Section 3.4.3.6.3).

Transposing operations are marked in this chapter by a star, $\star$ (with five points), which should be distinguished from an asterisk, $*$ (with six points), used to denote operations or symmetry elements in reciprocal space. The same designation is used in the software *GI$\star$KoBo*-1 and in the tables in Kopský (2001). A prime, $'$, is often used to designate transposing (twin) operations (see Section 3.3.5; Curien & Le Corre, 1958; Curien & Donnay, 1959). We have reserved the prime for operations involving time inversion, as is customary in magnetism (see Chapter 1.5). This choice allows one to analyse domain structures in magnetic and magnetoelectric materials (see *e.g.* Přívratská & Janovec, 1997).

In connection with this, we invoke the notion of a *twin law*. Since this term is not yet common in the context of domain structures, we briefly explain its meaning.

In crystallography, a twin is characterized by a twin law defined in the following way (see Section 3.3.2; Koch, 1999; Cahn, 1954):

(i) A *twin law* describes the geometrical relation between twin components of a twin. This relation is expressed by a *twin operation* that brings one of the twin components into parallel orientation with the other, and *vice versa*. A symmetry element corresponding to the twin operation is called the *twin element*. (Requirement 'and *vice versa*' is included in the definition of Cahn but not in that of Koch; for the most common twin operations of the second order the '*vice versa*' condition is fulfilled automatically.)

(ii) The relation between twin components deserves the name 'twin law' only if it occurs frequently, is reproducible and represents an inherent feature of the crystal.

An analogous definition of a *domain twin law* can be formulated for domain twins by replacing the term 'twin components' by 'domains', say $\mathbf{D}_i(\mathbf{S}_j, B_k)$ and $\mathbf{D}_m(\mathbf{S}_n, B_p)$, where $\mathbf{S}_j$, B_k and $\mathbf{S}_n$, B_p are, respectively, the domain state and the domain region of the domains $\mathbf{D}_i(\mathbf{S}_j, B_k)$ and $\mathbf{D}_m(\mathbf{S}_n, B_p)$, respectively (see Section 3.4.2.1). The term 'transposing operation' corresponds to transposing operation $g_{12}^\star$ of domain pair $(\mathbf{S}_1, \mathbf{S}_2) = (\mathbf{S}_j, g_{jn}^\star\mathbf{S}_n)$ as we have defined it above if two domains with domain states $\mathbf{S}_1$ and $\mathbf{S}_2$ *coexist* along a domain wall of the domain twin.

Domain twin laws can be conveniently expressed by crystallographic groups. This specification is simpler for non-ferroelastic twins, where a twin law can be expressed by a dichromatic space group (see Section 3.4.3.5), whereas for ferroelastic twins with a compatible domain wall dichromatic layer groups are adequate (see Section 3.4.3.6.3).

Restriction (ii), formulated by Georges Friedel (1926) and explained in detail by Cahn (1954), expresses a necessity to exclude from considerations crystal aggregates (intergrowths) with approximate or accidental 'nearly exact' crystal components resembling twins (Friedel's *macles d'imagination*) and thus to restrict the definition to 'true twins' that fulfil condition (i) exactly and are characteristic for a given material. If we confine our considerations to domain structures that are formed from a *homogeneous* parent phase, this requirement is fulfilled for *all* aggregates consisting of two or more domains. Then the definition of a 'domain twin law' is expressed only by condition (i). Condition (ii) is important for growth twins.

We should note that the definition of a twin law given above involves only domain states and does not explicitly contain
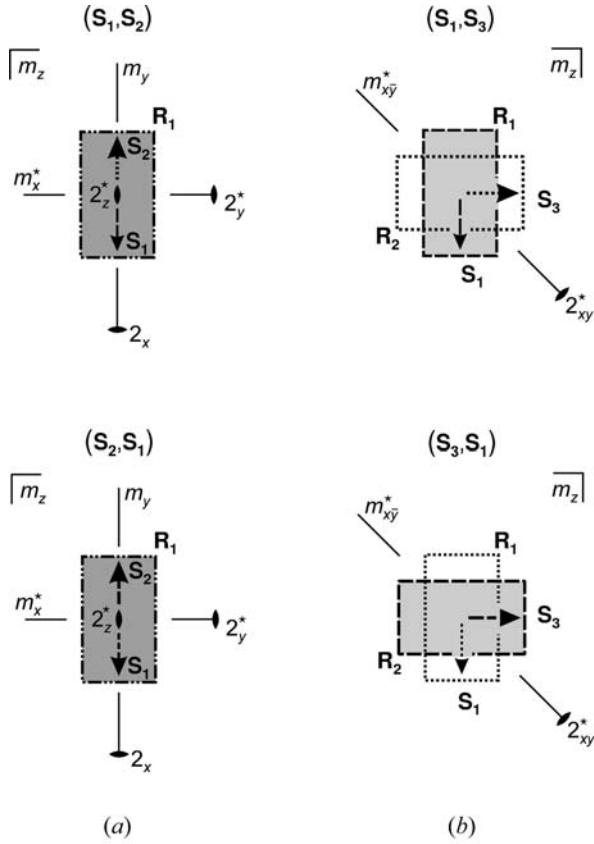
Fig. 3.4.3.1. Transposable domain pairs. Single-domain states are those from Fig. 3.4.2.2. (*a*) Completely transposable non-ferroelastic domain pair. (*b*) Partially transposable ferroelastic domain pair.

Fig. 3.4.3.2. Non-transposable domain pairs. (*a*) The parent phase with symmetry $G = 6_z/m_z$ is represented by a dotted hexagon and the three ferroelastic single-domain states with symmetry $F_1 = F_2 = F_3 = 2_z/m_z$ are depicted as drastically squeezed hexagons. (*b*) Domain pair $(\mathbf{S}_1, \mathbf{S}_2)$ and transposed domain pair $(\mathbf{S}_2, \mathbf{S}_1)$. There exists no operation from the group $6_z/m_z$ that would exchange domain states $\mathbf{S}_1$ and $\mathbf{S}_2$, *i.e.* that would transform one domain pair into a transposed domain pair.

specification of the contact region between twin components or neighbouring domains. The concept of domain state is, therefore, relevant for discussing the twin laws. Moreover, there is no requirement on the coexistence of interpenetrating structures in a domain pair. One can even, therefore, consider cases where no real coexistence of both structures is possible. Nevertheless, we note that the characterization of twin laws used in mineralogy often includes specification of the contact region (*e.g.* twin plane or diffuse region in penetrating twins).

Ordered domain pairs $(\mathbf{S}_1, \mathbf{S}_2)$ and $(\mathbf{S}_1, \mathbf{S}_3)$, formed from domain states of our illustrative example (see Fig. 3.4.2.2), are displayed in Fig. 3.4.3.1(*a*) and (*b*), respectively, as two superposed rectangles with arrows representing spontaneous polarization. In ordered domain pairs, the first and the second domain state are distinguished by shading [the first domain state is grey ('black') and the second clear ('white')] and/or by using dashed and dotted lines for the first and second domain state, respectively.

In Fig. 3.4.3.2, the ordered domain pair $(\mathbf{S}_1, \mathbf{S}_2)$ and the transposed domain pair $(\mathbf{S}_2, \mathbf{S}_1)$ are depicted in a similar way for another example with symmetry descent $G = 6_z/m_z \supset 2_z/m_z = F_1$.

Let us now examine the *symmetry of domain pairs*. The *symmetry group* F_{ik} *of an ordered domain pair* $(\mathbf{S}_i, \mathbf{S}_k) = (\mathbf{S}_i, g_{ik}\mathbf{S}_i)$ consists of all operations that leave invariant both $\mathbf{S}_i$ and $\mathbf{S}_k$, *i.e.* F_{ik} comprises all operations that are common to stabilizers (symmetry groups) F_i and F_k of domain states $\mathbf{S}_i$ and $\mathbf{S}_k$, respectively,

$$F_{ik} \equiv F_i \cap F_k = F_i \cap g_{ik} F_i g_{ik}^{-1}, \qquad (3.4.3.8)$$

where the symbol $\cap$ denotes the intersection of groups F_i and F_k. The group F_{ik} is in Section 3.3.4 denoted by $\mathcal{H}^*$ and is called an intersection group.
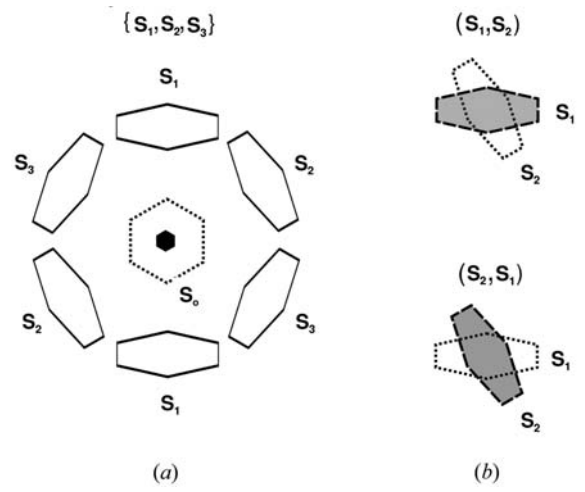
From equation (3.4.3.8), it immediately follows that the symmetry F_{ki} of the transposed domain pair $(\mathbf{S}_k, \mathbf{S}_i)$ is the same as the symmetry F_{ik} of the initial domain pair $(\mathbf{S}_i, \mathbf{S}_k)$:

$$F_{ki} = F_k \cap F_i = F_i \cap F_k = F_{ik}. \qquad (3.4.3.9)$$

Symmetry operations of an unordered domain pair $\{\mathbf{S}_i, \mathbf{S}_k\}$ include, besides operations of F_{ik} that do not change either $\mathbf{S}_i$ or $\mathbf{S}_k$, all transposing operations, since for an unordered domain pair a transposed domain pair is identical with the initial domain pair [see equation (3.4.3.4)]. If $g_{ik}^\star$ is a transposing operation of $(\mathbf{S}_i, \mathbf{S}_k)$, then all operations from the left coset $g_{ik}^\star F_{ik}$ are transposing operations of that domain pair as well. Thus the *symmetry group* J_{ik} *of an unordered domain pair* $\{\mathbf{S}_i, \mathbf{S}_k\}$ can be, in a general case, expressed in the following way:

$$J_{ik} = F_{ik} \cup g_{ik}^\star F_{ik}, \quad g_{ik}^\star \in G. \qquad (3.4.3.10)$$

Since, for an unordered domain, the order of domain states in a domain pair is not significant, the transposition of indices i, k in J_{ik} does not change this group,

$$J_{ik} = F_{ik} \cup g_{ik}^\star F_{ik} = F_{ki} \cup g_{ki}^\star F_{ki} = J_{ki}, \qquad (3.4.3.11)$$

which also follows from equations (3.4.3.3) and (3.4.3.9).

A *basic classification of domain pairs* follows from their symmetry. Domain pairs for which at least one transposing operation exists are called *transposable* (or *ambivalent*) *domain pairs*. The symmetry group of a transposable unordered domain pair $(\mathbf{S}_i, \mathbf{S}_k)$ is given by equation (3.4.3.10).

The star in the symbol $J_{ik}^\star$ indicates that this group contains transposing operations, *i.e.* that the corresponding domain pair $(\mathbf{S}_i, \mathbf{S}_k)$ is a transposable domain pair.

A transposable domain pair $(\mathbf{S}_i, \mathbf{S}_k)$ and transposed domain pair $(\mathbf{S}_k, \mathbf{S}_i)$ belong to the same G-orbit:

$$G(\mathbf{S}_i, \mathbf{S}_k) = G(\mathbf{S}_k, \mathbf{S}_i). \qquad (3.4.3.12)$$

If $\{\mathbf{S}_i, \mathbf{S}_k\}$ is a transposable pair and, moreover, $F_i = F_k = F_{ik}$, then *all* operations of the left coset $g_{ik}^\star F_i$ simultaneously switch $\mathbf{S}_i$ into $\mathbf{S}_k$ and $\mathbf{S}_k$ into $\mathbf{S}_i$. We call such a pair a *completely transposable domain pair*. The symmetry group J_{ik} of a completely transposable pair $\{\mathbf{S}_i, \mathbf{S}_k\}$ is

$$J_{ik}^\star = F_i \cup g_{ik}^\star F_i, \quad g_{ik}^\star \in G, \quad F_i = F_k. \qquad (3.4.3.13)$$

We shall use for symmetry groups of completely transposable domain pairs the symbol $J^\star_{ik}$.

If $F_i \neq F_k$, then $F_{ik} \subset F_i$ and the number of transposing operations is smaller than the number of operations switching $\mathbf{S}_i$ into $\mathbf{S}_k$. We therefore call such pairs *partially transposable domain pairs*. The symmetry group J_{ik} of a partially transposable domain pair $\{\mathbf{S}_i, \mathbf{S}_k\}$ is given by equation (3.4.3.10).

The symmetry groups J_{ik} and $J^\star_{ik}$, expressed by (3.4.3.10) or by (3.4.3.13), respectively, consists of two left cosets only. The first is equal to F_{ik} and the second one $g^\star_{ik} F_{ik}$ comprises all the transposing operations marked by a star. An explicit symbol $J_{ik}[F_{ik}]$ of these groups contains both the group J_{ik} and F_{ik}, which is a subgroup of J_{ik} of index 2.

If one 'colours' one domain state, *e.g.* $\mathbf{S}_i$, 'black' and the other, *e.g.* $\mathbf{S}_k$, 'white', then the operations without a star can be interpreted as 'colour-preserving' operations and operations with a star as 'colour-exchanging' operations. Then the group $J_{ik}[F_{ik}]$ can be treated as a 'black-and-white' or dichromatic group (see Section 3.2.3.2.7). These groups are also called Shubnikov groups (Bradley & Cracknell, 1972), two-colour or Heesch–Shubnikov groups (Opechowski, 1986), or antisymmetry groups (Vainshtein, 1994).

The advantage of this notation is that instead of an explicit symbol $J_{ik}[F_{ik}]$, the symbol of a dichromatic group specifies both the group J_{ik} and the subgroup F_{ij} or F_1, and thus also the transposing operations that define, according to equation (3.4.3.7), the second domain state $\mathbf{S}_j$ of the pair.

We have agreed to use a special symbol $J^\star_{ik}$ only for completely transposable domain pairs. Then the star in this case indicates that the subgroup F_{ik} is equal to the symmetry group of the first domain state $\mathbf{S}_i$ in the pair, $F_{ik} = F_i$. Since the group F_i is usually well known from the context (in our main tables it is given in the first column), we no longer need to add it to the symbol of J_{ik}.

Domain pairs for which an exchanging operation $g^\star_{ik}$ cannot be found are called *non-transposable* (or *polar*) *domain pairs*. The symmetry J_{ij} of a non-transposable domain pair is reduced to the usual 'monochromatic' symmetry group F_{ik} of the corresponding ordered domain pair $(\mathbf{S}_i, \mathbf{S}_k)$. The G-orbits of mutually transposed polar domain pairs are disjoint (Janovec, 1972):

$$G(\mathbf{S}_i, \mathbf{S}_k) \cap G(\mathbf{S}_k, \mathbf{S}_i) = \emptyset. \qquad (3.4.3.14)$$

Transposed polar domain pairs, which are always non-equivalent, are called *complementary domain pairs*.

If, in particular, $F_{ik} = F_i = F_k$, then the symmetry group of the unordered domain pair is

$$J_{ik} = F_i = F_k. \qquad (3.4.3.15)$$

In this case, the unordered domain pair $\{\mathbf{S}_i, \mathbf{S}_k\}$ is called a *non-transposable simple domain pair*.

If $F_i \neq F_k$, then the number of operations of F_{ik} is smaller than that of F_i and the symmetry group J_{ik} is equal to the symmetry group F_{ik} of the ordered domain pair $(\mathbf{S}_i, \mathbf{S}_k)$,

$$J_{ik} = F_{ik}, \quad F_{ik} \subset F_i. \qquad (3.4.3.16)$$

Such an unordered domain pair $\{\mathbf{S}_i, \mathbf{S}_k\}$ is called a *non-transposable multiple domain pair*. The reason for this designation will be given later in this section.

We stress that domain states forming a domain pair are not restricted to single-domain states. Any two domain states with a defined orientation in the coordinate system of the parent phase can form a domain pair for which all definitions given above are applicable.

Example 3.4.3.1. Now we examine domain pairs in our illustrative example of a phase transition with symmetry descent $G = 4_z/m_z m_x m_{xy} \supset 2_x m_y m_z = F_1$ and with four single-domain states $\mathbf{S}_1$, $\mathbf{S}_2$, $\mathbf{S}_3$ and $\mathbf{S}_3$, which are displayed in Fig. 3.4.2.2. The domain pair $\{\mathbf{S}_1, \mathbf{S}_2\}$ depicted in Fig. 3.4.3.1(*a*) is a completely transposable domain pair since transposing operations exist, *e.g.* $g^\star_{12} = m^\star_x$, and the symmetry group F_{12} of the ordered domain pair $(\mathbf{S}_1, \mathbf{S}_2)$ is

$$F_{12} = F_1 \cap F_2 = F_1 = F_2 = 2_x m_y m_z. \qquad (3.4.3.17)$$

The symmetry group J_{12} of the unordered pair $\{\mathbf{S}_1, \mathbf{S}_2\}$ is a dichromatic group,

$$J^\star_{12} = 2_x m_y m_z \cup m^\star_x\{2_x m_y m_z\} = m^\star_x m_y m_z. \qquad (3.4.3.18)$$

The domain pair $\{\mathbf{S}_1, \mathbf{S}_3\}$ in Fig. 3.4.3.1(*b*) is a partially transposable domain pair, since there are operations exchanging domain states $\mathbf{S}_1$ and $\mathbf{S}_3$, *e.g.* $g^\star_{13} = m^\star_{x\bar{y}}$, but the symmetry group F_{13} of the ordered domain pair $(\mathbf{S}_1, \mathbf{S}_3)$ is smaller than F_1:

$$F_{13} = F_1 \cap F_3 = 2_x m_y m_z \cap m_x 2_y m_z = \{1, m_z\} \equiv \{m_z\}, \qquad (3.4.3.19)$$

where 1 is an identity operation and $\{1, m_z\}$ denotes the group m_z. The symmetry group of the unordered domain pair $\{\mathbf{S}_1, \mathbf{S}_3\}$ is equal to a dichromatic group,

$$J_{13} = \{m_z\} \cup 2^\star_{xy}.\{m_z\} = 2^\star_{xy} m^\star_{\bar{x}y} m_z. \qquad (3.4.3.20)$$

The domain pair $(\mathbf{S}_1, \mathbf{S}_2)$ in Fig. 3.4.3.2(*b*) is a non-transposable simple domain pair, since there is no transposing operation of $G = 6_z/m_z$ that would exchange domain states $\mathbf{S}_1$ and $\mathbf{S}_2$, and $F_1 = F_2 = 2_z/m_z$. The symmetry group J_{12} of the unordered domain pair $\{\mathbf{S}_1, \mathbf{S}_3\}$ is a 'monochromatic' group,

$$J_{12} = F_{12} = F_1 = F_2 = 2_z/m_z. \qquad (3.4.3.21)$$

The G-orbit $6_z/m_z(\mathbf{S}_1, \mathbf{S}_2)$ of the pair $(\mathbf{S}_1, \mathbf{S}_2)$ has no common domain pair with the G-orbit $6_z/m_z(\mathbf{S}_2, \mathbf{S}_1)$ of the transposed domain pair $(\mathbf{S}_2, \mathbf{S}_1)$. These two 'complementary' orbits contain mutually transposed domain pairs.

Symmetry groups of domain pairs provide a basic classification of domain pairs into the four types introduced above. This classification applies to microscopic domain pairs as well.

3.4.3.2. *Twinning group, distinction of two domain states*

We have seen that for transposable domain pairs the symmetry group J_{1j} of a domain pair $(\mathbf{S}_1, \mathbf{S}_j)$ specifies transposing operations $g^\star_{1j} F_1$ that transform $\mathbf{S}_1$ into $\mathbf{S}_j$. This does not apply to non-transposable domain pairs, where the symmetry group $J_{1j} = F_{1j}$ does not contain any switching operation. Another group exists, called the twinning group, which is associated with a domain pair and which does not have this drawback. The twinning group determines the distinction of two domain states, specifies the external fields needed to switch one domain state into another one and enables one to treat domain pairs independently of the transition $G \supset F_1$. This facilitates the tabulation of the properties of non-equivalent domain pairs that appear in all possible ferroic phases.

The *twinning group* K_{1j} of a *domain pair* $(\mathbf{S}_1, \mathbf{S}_j)$ is defined as the *minimal* subgroup of G that contains both F_1 and a switching operation g_{1j} of the domain pair $(\mathbf{S}_1, \mathbf{S}_j)$, $\mathbf{S}_j = g_{1j}\mathbf{S}_1$ (Fuksa & Janovec, 1995; Janovec *et al.*, 1995; Fuksa, 1997),

$$F_1 \subset K_{1j} \subseteq G, \quad g_{1j} \in K_{1j}, \qquad (3.4.3.22)$$

where no group K'_{1j} exists such that

$$F_1 \subset K'_{1j} \subset K_{1j}, \quad g_{1j} \in K'_{1j}. \qquad (3.4.3.23)$$

The twinning group K_{1j} is identical to the embracing (fundamental) group used in bicrystallography (see Section 3.2.2). In Section 3.3.4 it is called a composite symmetry of a twin.

Since K_{1j} is a group, it must contain all products of g_{1j} with operations of F_1, *i.e.* the whole left coset $g_{1j}F_1$. For completely transposable domain pairs, the union of F_1 and $g_{1j}^\star F_1$ forms a group that is identical with the symmetry group $J_{1j}^\star$ of the unordered domain pair $\{\mathbf{S}_1, \mathbf{S}_j\}$:

$$K_{1j}^\star = J_{1j}^\star = F_1 \cup g_{1j}^\star F_1, \quad g_{1j}^\star \in K_{1j}, \quad F_1 = F_j. \quad (3.4.3.24)$$

In a general case, the twinning group K_{1j}, being a supergroup of F_1, can always be expressed as a decomposition of the left cosets of F_1,

$$K_{1j} = F_1 \cup g_{1j}F_1 \cup g_{1k}F_1 \cup \ldots \cup g_{1c} \in G. \quad (3.4.3.25)$$

We can associate with the twinning group a set of c domain states, the K_{1j}-orbit of $\mathbf{S}_1$, which can be generated by applying to $\mathbf{S}_1$ the representatives of the left cosets in decomposition (3.4.3.25),

$$K_{1j}\mathbf{S}_1 = \{\mathbf{S}_1, \mathbf{S}_j, \ldots, \mathbf{S}_c\}. \quad (3.4.3.26)$$

This orbit is called the *generic orbit of domain pair* $(\mathbf{S}_1, \mathbf{S}_j)$.

Since the generic orbit (3.4.3.26) contains both domain states of the domain pair $(\mathbf{S}_1, \mathbf{S}_j)$, one can find different and equal nonzero *tensor components in two domain states* $\mathbf{S}_1$ and $\mathbf{S}_j$ by a similar procedure to that used in Section 3.4.2.3 for ascribing principal and secondary tensor parameters to principal and secondary domain states. All we have to do is just replace the group G of the parent phase by the twinning group K_{1j}. There are, therefore, three kinds of nonzero tensor components in $\mathbf{S}_1$ and $\mathbf{S}_j$:

(1) Domain states $\mathbf{S}_1$ and $\mathbf{S}_j$ differ in the principal tensor parameters κ_a of the 'virtual' phase transition with symmetry descent $K_{1j} \supset F_1$,

$$\kappa_a^{(1)} \neq \kappa_a^{(j)}, \quad a = 1, 2, \ldots, \quad (3.4.3.27)$$

where $\kappa_a^{(1)}$ and $\kappa_a^{(j)}$ are the principal tensor parameters in domain states $\mathbf{S}_1$ and $\mathbf{S}_j$; in the symbol of the principal tensor parameter κ_a we explicitly write only the lower index a, which numbers different principal tensor parameters, but omit the upper index labelling the representation of K_{1j}, according to which κ_a transforms, and the second lower index denoting the components of the principal tensor parameter (see Section 3.4.2.3 and the manual of the software *GI*★*KoBo*-1, path: *Subgroups\View\Domains* and Kopský, 2001).

The principal tensor parameters $\kappa_a^{(1)}$ of lower rank in domain state $\mathbf{S}_1$ can be found for $G = K_{1j}$ in Table 3.1.3.1 of Section 3.1.3.3, where we replace G by K_{1j}, and for all important property tensors in the software *GI*★*KoBo*-1, path: *Subgroups\View\Domains* and in Kopský (2001), where we again replace G by K_{1j}. Tensor parameters in domain state $\mathbf{S}_j$ can be obtained by applying to the principal tensor parameters in $\mathbf{S}_1$ the operation g_{1j}.

(2) If there exists an intermediate group L_{1j} in between F_1 and K_{1j} that does not – contrary to K_{1j} – contain the switching operation g_{1j} of the domain pair $(\mathbf{S}_1, \mathbf{S}_j)$,

$$F_1 \subset L_{1j} \subseteq K_{1j}, \quad g_{1j} \in L_{1j}, \quad (3.4.3.28)$$

[*cf.* relation (3.4.3.23)] then domain states $\mathbf{S}_1$ and $\mathbf{S}_j$ differ not only in the principal tensor parameters κ_a, but also in the secondary tensor parameters λ_b:

$$\lambda_b^{(1)} \neq \lambda_b^{(j)}, \quad I_{K_{1j}}(\lambda_b^{(1)}) = L_{1j}, \quad b = 1, \ldots, \quad (3.4.3.29)$$

where $\lambda_b^{(1)}$ and $\lambda_b^{(j)}$ are the secondary tensor parameters in domain states $\mathbf{S}_1$ and $\mathbf{S}_j$; the last equation, in which $I_{K_{1j}}(\lambda_b^{(1)})$ is the stabilizer of $\lambda_b^{(1)}$ in K_{1j}, expresses the condition that λ_b is the principal tensor parameter of the transition $K_{1j} \supset L_{1j}$ [see equation (3.4.2.40)].

The secondary tensor parameters $\lambda_b^{(1)}$ of lower rank in domain state $\mathbf{S}_1$ can be found for $G = K_{1j}$ in Table 3.1.3.1 of Section

3.1.3.3, and for all important property tensors in the software *GI*★*KoBo*-1, path: *Subgroups\View\Domains* and in Kopský (2001). Tensor parameters $\lambda_b^{(j)}$ in domain state $\mathbf{S}_j$ can be obtained by applying to the secondary tensor parameters $\lambda_b^{(1)}$ in $\mathbf{S}_1$ the operation g_{1j}.

(3) All nonzero tensor components that are the same in domain states $\mathbf{S}_1$ and $\mathbf{S}_j$ are identical with nonzero tensor components of the group K_{1j}. These components are readily available for all important material tensors in Section 1.1.4, in the software *GI*★*KoBo*-1, path: *Subgroups\View\Domains* and in Kopský (2001).

Cartesian tensor components corresponding to the tensor parameters can be calculated by means of conversion equations [for details see the manual of the software *GI*★*KoBo*-1, path: *Subgroups\View\Domains* and Kopský (2001)].

Let us now illustrate the above recipe for finding tensor distinctions by two simple examples.

Example 3.4.3.2. The domain pair $(\mathbf{S}_1, \mathbf{S}_2)$ in Fig. 3.4.3.1(*a*) is a completely transposable pair, therefore, according to equations (3.4.3.24) and (3.4.3.18),

$$K_{12}^\star = J_{12}^\star = 2_x m_y m_z \cup m_x^\star\{2_x m_y m_z\} = m_x^\star m_y m_z. \quad (3.4.3.30)$$

In Table 3.1.3.1, we find that the first principal tensor parameter $\kappa^{(1)}$ of the transition $G = K_{1j} = m_x m_y m_z \supset 2_x m_y m_z = F_1$ is the x-component P_1 of the spontaneous polarization, $\kappa_1^{(1)} = P_1$. Since the switching operation $g_{12}^\star$ is for example the inversion $\bar{1}$, the tensor parameter $\kappa_1^{(2)}$ in the second domain state $\mathbf{S}_2$ is $\kappa_1^{(2)} = -P_1$.

Other principal tensor parameters can be found in the software *GI*★*KoBo*-1 or in Kopský (2001), p. 185. They are: $\kappa_2^{(1)} = d_{12}$, $\kappa_3^{(1)} = d_{13}$, $\kappa_4^{(1)} = d_{26}$, $\kappa_5^{(1)} = d_{35}$ (the physical meaning of the components is explained in Table 3.4.3.5). In the second domain state $\mathbf{S}_2$, these components have the opposite sign. No other tensor components exist that would be different in $\mathbf{S}_1$ and $\mathbf{S}_2$, since there is no intermediate group L_{1j} in between F_1 and K_{1j}.

Nonzero components that are the same in both domain states are nonzero components of property tensors in the group mmm and are listed in Section 1.1.4.7 or in the software *GI*★*KoBo*-1 or in Kopský (2001).

The numbers of independent tensor components that are different and those that are the same in two domain states are readily available for all non-ferroelastic domain pairs and important property tensors in Table 3.4.3.4.

Example 3.4.3.3. The twinning group of the partially transposable domain pair $(\mathbf{S}_1, \mathbf{S}_3)$ in Fig. 3.4.3.1(*b*) with $\mathbf{S}_3 = 2_{xy}\mathbf{S}_1$ has the twinning group

$$K_{13} = 2_x m_y m_z \cup 2_{xy}\{2_x m_y m_z\} \cup 2_z\{2_x m_y m_z\} \cup 2_{x\bar{y}}\{2_x m_y m_z\}$$
$$= 4_z/m_z m_x m_{xy}. \quad (3.4.3.31)$$

Domain states $\mathbf{S}_1$ and $\mathbf{S}_3$ differ in the principal tensor parameter of the transition $4_z/m_z m_x m_{xy} \subset 2_x m_y m_z$, which is two-dimensional and which we found in Example 3.4.2.4: $\kappa_1^{(1)} = (P, 0)$. Then in the domain state $\mathbf{S}_3$ it is $\kappa_1^{(3)} = D(2_{xy})(P, 0) = (0, P)$. Other principal tensors are: $\kappa_2^{(1)} = (g_4, 0)$, $\kappa_3^{(1)} = (d_{11}, 0)$, $\kappa_4^{(1)} = (d_{12}, 0)$, $\kappa_5^{(1)} = (d_{13}, 0)$, $\kappa_6^{(1)} = (d_{26}, 0)$, $\kappa_7^{(1)} = (d_{35}, 0)$ (the physical meaning of the components is explained in Table 3.4.3.5). In the domain state $\mathbf{S}_3$ they keep their absolute value but appear as the second nonzero components, as with spontaneous polarization.

There is an intermediate group $L_{13} = m_x m_y m_z$ between $F_1 = 2_x m_y m_z$ and $K_{13} = 4_z/m_z m_x m_{xy}$, since $L_{13} = m_x m_y m_z$ does not contain $g_{13} = 2_{xy}$. The one-dimensional secondary tensor parameters for the symmetry descent $K_{13} = 4_z/m_z m_x m_{xy} \supset L_{13} = m_x m_y m_z$ was also found in Example 3.4.2.4: $\lambda_1^{(1)} = u_1 - u_2$;

$\lambda_2^{(1)} = A_{14} + A_{25}, A_{36}; \quad \lambda_3^{(1)} = s_{11} - s_{22}, \quad s_{13} - s_{23}, \quad s_{44} - s_{55};$
$\lambda_4^{(1)} = Q_{11} - Q_{22}, Q_{12} - Q_{21}, Q_{13} - Q_{23}, Q_{31} - Q_{32}, Q_{44} - Q_{55}.$
All these parameters have the opposite sign in $\mathbf{S}_3$.

The tensor distinction of two domain states $\mathbf{S}_1$ and $\mathbf{S}_j$ in a domain pair $(\mathbf{S}_1, \mathbf{S}_j)$ provides a useful *classification of domain pairs* given in the second and the third columns of Table 3.4.3.1. This classification can be extended to ferroic phases which are named according to domain pairs that exist in this phase. Thus, for example, if a ferroic phase contains ferroelectric (ferroelastic) domain pair(s), then this phase is a ferroelectric (ferroelastic) phase. Finer division into full and partial ferroelectric (ferroelastic) phases specifies whether all or only some of the possible domain pairs in this phase are ferroelectric (ferroelastic) ones. Another approach to this classification uses the notions of principal and secondary tensor parameters, and was explained in Section 3.4.2.2.

A discussion of and many examples of secondary ferroic phases are available in papers by Newnham & Cross (1974*a*,*b*) and Newnham & Skinner (1976), and tertiary ferroic phases are discussed by Amin & Newnham (1980).

We shall now show that the tensor distinction of domain states is closely related to the switching of domain states by external fields.

3.4.3.3. *Switching of ferroic domain states*

We saw in Section 3.4.2.1 that all domain states of the orbit $G\mathbf{S}_1$ have the same chance of appearing. This implies that they have the same free energy, *i.e.* they are degenerate. The same conclusion follows from thermodynamic theory, where domain states appear as equivalent solutions of equilibrium values of the order parameter, *i.e.* all domain states exhibit the same free energy Ψ (see Section 3.1.2). These statements hold under a tacit assumption of absent external electric and mechanical fields. If these fields are nonzero, the degeneracy of domain states can be partially or completely lifted.

The free energy $\Psi^{(k)}$ per unit volume of a ferroic domain state $\mathbf{S}_k$, $k = 1, 2, \ldots, n$, with spontaneous polarization $\mathbf{P}_0^{(k)}$ with components $P_{0i}^{(k)}$, $i = 1, 2, 3$, and with spontaneous strain components $u_{0\mu}^{(k)}$, $\mu = 1, 2, \ldots, 6$, is (Aizu, 1972)

$$\Psi^{(k)} = \Psi_0 - P_{0i}^{(k)}E_i - u_{0\mu}^{(k)}\sigma_\mu - d_{i\mu}^{(k)}E_i\sigma_\mu - \tfrac{1}{2}\varepsilon_0\kappa_{ik}^{(k)}E_iE_k$$
$$- \tfrac{1}{2}s_{\mu\nu}^{(k)}\sigma_\mu\sigma_\nu - \tfrac{1}{2}Q_{ik\mu}^{(k)}E_iE_k\sigma_\mu - \ldots, \qquad (3.4.3.32)$$

where the Einstein summation convention (summation with respect to suffixes that occur twice in the same term) is used with $i, j = 1, 2, 3$ and $\mu, \nu = 1, 2, \ldots, 6$. The symbols in equation (3.4.3.32) have the following meaning: E_i and u_μ are components of the external electric field and of the mechanical stress, respectively, $d_{i\mu}^{(k)}$ are components of the piezoelectric tensor, $\varepsilon_0\kappa_{ij}^{(k)}$ are components of the electric susceptibility, $s_{\mu\nu}^{(k)}$ are

compliance components, and $Q_{ij\mu}^{(k)}$ are components of electrostriction (components with Greek indices are expressed in matrix notation) [see Section 3.4.5 (Glossary), Chapter 1.1 or Nye (1985); Sirotin & Shaskolskaya (1982)].

We shall examine two domain states $\mathbf{S}_1$ and $\mathbf{S}_j$, *i.e.* a domain pair $(\mathbf{S}_1, \mathbf{S}_j)$, in electric and mechanical fields. The difference of their free energies is given by

$$\Psi^{(j)} - \Psi^{(1)} = -(P_{0i}^{(j)} - P_{0i}^{(1)})E_i - (u_{0\mu}^{(j)} - u_{0\mu}^{(1)})\sigma_\mu - (d_{i\mu}^{(j)} - d_{i\mu}^{(1)})E_i\sigma_\mu$$
$$- \tfrac{1}{2}\varepsilon_0(\kappa_{ik}^{(j)} - \kappa_{ik}^{(1)})E_iE_k - \tfrac{1}{2}(s_{\mu\nu}^{(j)} - s_{\mu\nu}^{(1)})\sigma_\mu\sigma_\nu$$
$$- \tfrac{1}{2}(Q_{ik\mu}^{(j)} - Q_{ik\mu}^{(1)})E_iE_k\sigma_\mu - \ldots. \qquad (3.4.3.33)$$

For a domain pair $(\mathbf{S}_1, \mathbf{S}_j)$ and given external fields, there are three possibilities:

(1) $\Psi^{(j)} = \Psi^{(1)}$. Domain states $\mathbf{S}_1$ and $\mathbf{S}_j$ can coexist in equilibrium in given external fields.

(2) $\Psi^{(j)} < \Psi^{(1)}$. In given external fields, domain state $\mathbf{S}_j$ is more stable than $\mathbf{S}_1$; for large enough fields (higher than the coercive ones), the state $\mathbf{S}_1$ switches into the state $\mathbf{S}_j$.

(3) $\Psi^{(j)} > \Psi^{(1)}$. In given external fields, domain state $\mathbf{S}_j$ is less stable than $\mathbf{S}_1$; for large enough fields (higher than the coercive ones), the state $\mathbf{S}_j$ switches into the state $\mathbf{S}_1$.

A typical dependence of applied stress and corresponding strain in ferroelastic materials has a form of a elastic hysteresis loop (see Fig. 3.4.1.3). Similar dielectric hysteresis loops are observed in ferroelectric materials; examples can be found in books on ferroelectric crystals (*e.g.* Jona & Shirane, 1962).

A classification of switching (state shifts in Aizu's terminology) based on equation (3.4.3.33) was put forward by Aizu (1972, 1973) and is summarized in the second and fourth columns of Table 3.4.3.1. The order of the state shifts specifies the switching fields that are necessary for switching one domain state of a domain pair into the second state of the pair.

Another distinction related to switching distinguishes between *actual* and *potential* ferroelectric (ferroelastic) phases, depending on whether or not it is possible to switch the spontaneous polarization (spontaneous strain) by applying an electric field (mechanical stress) lower than the electrical (mechanical) breakdown limit under reasonable experimental conditions (Wadhawan, 2000). We consider in our classification always the potential ferroelectric (ferroelastic) phase.

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

Table 3.4.3.1. *Classification of domain pairs, ferroic phases and of switching (state shifts)*

$P_{0i}^{(k)}$ and $u_{0\mu}^{(k)}$ are components of the spontaneous polarization and spontaneous strain in the domain state $\mathbf{S}_k$, where $k = 1$ or $k = j$; similarly, $d_{i\mu}^{(k)}$ are components of the piezoelectric tensor, $\varepsilon_0\kappa_{ij}^{(k)}$ are components of electric susceptibility, $s_{\mu\nu}^{(k)}$ are compliance components and $Q_{ij\mu}^{(k)}$ are components of electrostriction (components with Greek indices are expressed in matrix notation) [see Chapter 1.1 or *e.g.* Nye (1985) and Sirotin & Shaskolskaya (1982)]. Text in italics concerns the classification of ferroic phases. $\mathbf{E}$ is the electric field and σ is the mechanical stress.

Ferroic class	Domain pair – *at least in one pair*	Domain pair – *phase*	Switching (state shift)	Switching field
Primary	At least one $P_{0i}^{(j)} - P_{0i}^{(1)} \neq 0$	Ferroelectric	Electrically first order	$\mathbf{E}$
	At least one $u_{0\mu}^{(j)} - u_{0\mu}^{(1)} \neq 0$	Ferroelastic	Mechanically first order	σ
Secondary	At least one $P_{0i}^{(j)} - P_{0i}^{(1)} \neq 0$ and at least one $u_{0\mu}^{(j)} - u_{0\mu}^{(1)} \neq 0$	Ferroelastoelectric	Electromechanically first order	$\mathbf{E}\sigma$
	All $P_{0i}^{(j)} - P_{0i}^{(1)} = 0$ and at least one $\varepsilon_0(\kappa_{ik}^{(j)} - \kappa_{ik}^{(1)}) \neq 0$	Ferrobielectric	Electrically second order	$\mathbf{EE}$
	All $u_{0\mu}^{(j)} - u_{0\mu}^{(1)} = 0$ and at least one $s_{\mu\nu}^{(j)} - s_{\mu\nu}^{(1)} \neq 0$	Ferrobielastic	Mechanically second order	$\sigma\sigma$
$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$

$i, j = 1, 2, 3; \mu, \nu = 1, 2, \ldots, 6.$

Table 3.4.3.2. *Four types of domain pairs*

F_{1j}	J_{1j}	K_{1j}	Double coset	Domain pair name symbol	
$F_1 = F_j$	$F_1 \cup g_{1j}^\star F_1$	$F_1 \cup g_{1j}^\star F_1$	$F_1 g_{1j} F_1 = g_{1j} F_1 = (g_{1j} F_1)^{-1}$	*t*ransposable *c*ompletely	tc
$F_{1j} \subset F_1$	$F_{1j} \cup g_{1j}^\star F_{1j}$	$F_1 \cup g_{1j}^\star F_1 \cup \ldots$	$F_1 g_{1j} F_1 = (F_1 g_{1j} F_1)^{-1}$	*t*ransposable *p*artially	tp
$F_1 = F_j$	F_1	$F_1 \cup g_{1j} F_1 \cup g_{1j}^{-1} F_1$	$F_1 g_{1j} F_1 = g_{1j} F_1 \cap (g_{1j} F_1)^{-1} = \emptyset$	*n*on-transposable *s*imple	ns
$F_{1j} \subset F_1$	F_{1j}	$F_1 \cup g_{1j} F_1 \cup (g_{1j} F_1)^{-1} \cup \ldots$	$F_1 g_{1j} F_1 \cap (F_1 g_{1j} F_1)^{-1} = \emptyset$	*n*on-transposable *m*ultiple	nm

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

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

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

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

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

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

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

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

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

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

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

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

$$G(\mathbf{S}_1, \mathbf{S}_j) \leftrightarrow F_1 g_j F_1, \quad \text{where} \quad \mathbf{S}_j = g_j \mathbf{S}_1, \quad j = 1, 2, \ldots, q.$$
$$(3.4.3.36)$$

We see that the representatives g_j of the double cosets in decomposition (3.4.3.35) define domain pairs $(\mathbf{S}_1, g_j\mathbf{S}_1)$ which represent all different G-orbits of domain pairs. Just as different left cosets $g_i F_1$ specify all domain states, different double cosets determine all classes of equivalent domain pairs (G-orbits of domain pairs).

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

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

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

A double coset that is disjoint with its inverse,

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

is a *non-invertible (polar) double coset* ($\emptyset$ denotes an empty set) and the corresponding class of domain pairs comprises non-transposable (polar) domain pairs. A double coset $F_1 g_j F_1$ and its inverse $(F_1 g_j F_1)^{-1}$ are called *complementary double cosets*. Corresponding classes called *complementary classes of equivalent domain pairs* consist of transposed domain pairs that are non-equivalent.

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

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

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

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

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

When one applies operations from the first left coset on the third left coset, one gets the fourth left coset, therefore a double coset consists of these two left cosets. An inverse of any operation of this double coset belongs to this double coset, hence it is a multiple invertible double coset. Corresponding domain pairs are partially transposable ones. A representative pair is, for example,

Table 3.4.3.3. *Decomposition of $G = 6_z/m_z$ into left cosets of $F_1 = 2_z/m_z$*

Left coset				Principal domain state
1	2_z	$\bar{1}$	m_z	$\mathbf{S}_1$
3_z	6_z^5	$\bar{3}_z$	$\bar{6}_z^5$	$\mathbf{S}_2$
3_z^2	6_z	$\bar{3}_z^5$	$\bar{6}_z$	$\mathbf{S}_3$

$(\mathbf{S}_1, 2_{xy}\mathbf{S}_1) = (\mathbf{S}_1, \mathbf{S}_3)$ which is indeed a partially transposable domain pair [*cf.* (3.4.3.19) and (3.4.3.20)]. The class of equivalent ordered domain pairs is $(\mathbf{S}_1, \mathbf{S}_3) \overset{G}{\sim} (\mathbf{S}_3, \mathbf{S}_1) \overset{G}{\sim} (\mathbf{S}_1, \mathbf{S}_4) \overset{G}{\sim} (\mathbf{S}_4, \mathbf{S}_1) \overset{G}{\sim}$ $(\mathbf{S}_3, \mathbf{S}_2) \overset{G}{\sim} (\mathbf{S}_2, \mathbf{S}_3) \overset{G}{\sim} (\mathbf{S}_2, \mathbf{S}_4) \overset{G}{\sim} (\mathbf{S}_4, \mathbf{S}_2)$. These are '90° domain pairs'.

An example of non-invertible double cosets is provided by the decomposition of the group $G = 6_z/m_z$ into left and double cosets of $F_1 = 2_z/m_z$ displayed in Table 3.4.3.3. The inverse of the second left coset (second line) is equal to the third left coset (third line) and *vice versa*. Each of these two left cosets thus corresponds to a double coset and these double cosets are complementary double cosets. Corresponding representative simple non-transposable domain pairs are $(\mathbf{S}_1, \mathbf{S}_2)$ and $(\mathbf{S}_2, \mathbf{S}_1)$, and are depicted in Fig. 3.4.3.2.

We conclude that *double cosets determine classes of equivalent domain pairs that can appear in the ferroic phase resulting from a phase transition with a symmetry descent $G \supset F_1$*. Left coset and double coset decompositions for all crystallographic point-group descents are available in the software *GI⋆KoBo*-1, path: *Subgroups\View\Twinning groups*.

A double coset can be specified by any operation belonging to it. This representation is not very convenient, since it does not reflect the properties of corresponding domain pairs and there are many operations that can be chosen as representatives of a double coset. It turns out that in a continuum description the twinning group K_{1j} can represent classes of equivalent domain pairs $G(\mathbf{S}_1, \mathbf{S}_j)$ with two exceptions:

(i) Two complementary classes of non-transposable domain pairs have the same twinning group. This follows from the fact that if a twinning group contains the double coset, then it must comprise also the inverse double coset.

(ii) Different classes of transposable domain pairs have different twining groups except in the following case (which corresponds to the orthorhombic ferroelectric phase in perovskites): the group $F_1 = m_{x\bar{y}}2_{xy}m_z$ generates with switching operations $g = 2_{yz}$ and $g_3 = m_{yz}$ two different double cosets with the same twinning group $K_{12} = K_{13} = m\bar{3}m$ (one can verify this in the software *GI⋆KoBo*-1, path: *Subgroups\View\Twinning groups*). Domain states are characterized in this ferroelectric phase by the direction of the spontaneous polarization. The angles between the spontaneous polarizations of the domain states in domain pairs $(\mathbf{S}_1, 2_{yz}\mathbf{S}_1)$ and $(\mathbf{S}_1, m_{yz}\mathbf{S}_1)$ are 120 and 60°, respectively; this shows that these representative domain pairs are not equivalent and belong to two different 'G-orbits of domain pairs. To distinguish these two cases, we add to the twinning group $m\bar{3}m[m_{x\bar{y}}2_{xy}m_z]$ either the switching operation 2_{yz} or m_{yz}, *i.e.* the two distinct orbits are labelled by the symbols $m\bar{3}m(2_{xy})$ and $m\bar{3}m(m_{xy})$, respectively.

Bearing in mind these two exceptions, *one can, in the continuum description, represent G-orbits of domain pairs $G(\mathbf{S}_1, \mathbf{S}_j)$ by twinning groups $K_{1j}[F_1]$.*

We have used this correspondence in synoptic Table 3.4.2.7 of symmetry descents at ferroic phase transitions. For each symmetry descent $G \supset F_1$, the twinning groups given in column K_{1j} specify possible G-orbits of domain pairs that can appear in the domain structure of the ferroic phase (Litvin & Janovec, 1999). We divide all orbits of domain pairs (represented by corresponding twinning groups K_{1j}) that appear in Table 3.4.2.7 into classes of non-ferroelastic and ferroelastic domain pairs and present them with further details in the three synoptic Tables 3.4.3.4, 3.4.3.6 and 3.4.3.7 described in Sections 3.4.3.5 and 3.4.3.6.

As we have seen, a classification of domain pairs according to their internal symmetry (summarized in Table 3.4.3.2) introduces a partition of all domain pairs that can be formed from domain states of the G-orbit $G\mathbf{S}_1$ into equivalence classes of pairs with the same internal symmetry. Similarly, any inherent physical property of domain pairs induces a partition of all domain pairs into corresponding equivalence classes. Thus, for example, the

classification of domain pairs, based on tensor distinction or switching of domain states (see Table 3.4.3.1, columns two and three), introduces a division of domain pairs into corresponding equivalence classes.

3.4.3.5. *Non-ferroelastic domain pairs: twin laws, domain distinction and switching fields, synoptic table*

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

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

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

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

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

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

(Complete transposability is only a necessary, but not a sufficient, condition of a non-ferroelastic domain pair, since there are also ferroelastic domain pairs that are completely transposable – see Table 3.4.3.6.)

The relation between domain states in a non-ferroelastic domain twin, in which two domain states coexist, is the same as that of a corresponding non-ferroelastic domain pair consisting of *single-domain* states. Transposing operations $g_{1j}^\star$ are, therefore, also *twinning operations*.

Synoptic Table 3.4.3.4 lists representative domain pairs of all orbits of non-ferroelastic domain pairs. Each pair is specified by the first domain state $\mathbf{S}_1$ with symmetry group F_1 and by transposing operations $g_{1j}^\star$ that transform $\mathbf{S}_1$ into $\mathbf{S}_j$, $\mathbf{S}_j = g_{1j}^\star\mathbf{S}_1$. Twin laws in dichromatic notation are presented and basic data for tensor distinction and switching of non-ferroelastic domains are given.

3.4.3.5.1. *Explanation of Table 3.4.3.4*

The first three columns *specify domain pairs*.

F_1: *point-group symmetry (stabilizer in K_{1j}) of the first domain state $\mathbf{S}_1$) in a single-domain orientation*. There are two domain states with the same F_1; one has to be chosen as $\mathbf{S}_1$. Subscripts of generators in the group symbol specify their orientation in the Cartesian (rectangular) crystallophysical coordinate system of the group K_{1j} (see Tables 3.4.2.5, 3.4.2.6 and Figs. 3.4.2.3, 3.4.2.4).

$g_{1j}^\star$: *switching operations* that specify domain pair $(\mathbf{S}_1, g_{1j}^\star\mathbf{S}_1) = (\mathbf{S}_1, \mathbf{S}_j)$. Subscripts of symmetry operations specify the orientation of the corresponding symmetry element in the Cartesian (rectangular) crystallophysical coordinate system of the group K_{1j}. In hexagonal and trigonal systems, x', y' and x'', y'' denote the Cartesian coordinate system rotated about the z axis through 120 and 240°, respectively, from the Cartesian coordinate axes x and y; diagonal directions are abbreviated: $p = [111]$, $q = [\bar{1}11]$, $r = [1\bar{1}1]$, $s = [11\bar{1}]$ (for further details see Tables 3.4.2.5 and 3.4.2.6, and Figs. 3.4.2.3 and 3.4.2.4).

All switching operations of the second order are given, switching operations of higher order are omitted. The star symbol signifies that the operation is both a transposing and a twinning operation.

$K_{1j}^\star = J_{1j}^\star$: *twinning group of the domain pair* $(\mathbf{S}_1, \mathbf{S}_j)$. This group is equal to the symmetry group $J_{1j}^\star$ of the completely transposable unordered domain pair $\{\mathbf{S}_1, \mathbf{S}_j\}$ [see equation (3.4.3.24)]. The dichromatic symbol of the group $K_{1j}^\star = J_{1j}^\star$ designates the *twin law of the non-ferroelastic domain pair* $\{\mathbf{S}_1, \mathbf{S}_j\}$ and the *twin law of all*

Table 3.4.3.4. *Non-ferroelastic domain pairs, domain twin laws and distinction of non-ferroelastic domains*

F_1: symmetry of $\mathbf{S}_1$; $g_{1j}^\star$: twinning operations of second order; $K_{1j}^\star$: twinning group signifying the twin law of domain pair $(\mathbf{S}_1, g_{1j}^\star\mathbf{S}_1)$; $J_{1j}^\star$: symmetry group of the pair; Γ_α: irreducible representation of $K_{1j}^\star$; ϵ, $\mathbf{P}_i$, ..., $\mathbf{Q}_{ij\mu}$: components of property tensors (see Table 3.4.3.5): $a|c$: number of distinct|equal nonzero tensor components of property tensors.

F_1	$g_{1j}^\star$	$K_{1j}^\star = J_{1j}^\star$	Γ_α	Diffraction intensities	ϵ	$\mathbf{P}_i$	g_μ	$d_{i\mu}$	$A_{i\mu}$	$s_{\mu\nu}$	$\mathbf{Q}_{ij\mu}$
1	$\bar{1}^\star$	$\bar{1}^\star$	A_u	=	1|0	3|0	6|0	18|0	0|18	0|21	0|36
2_u†	$\bar{1}^\star, m_u^\star$	$2_u/m_u^\star$	A_u	=	1|0	1|0	4|0	8|0	0|8	0|13	0|20
m_u†	$\bar{1}^\star, 2_u^\star$	$2_u^\star/m_u$	B_u	=	0|0	2|0	2|0	10|0	0|8	0|13	0|20
$2_x2_y2_z$	$\bar{1}^\star, m_x^\star, m_y^\star, m_z^\star$	$m_x^\star m_y^\star m_z^\star$	A_u	=	1|0	0|0	3|0	3|0	0|3	0|9	0|12
$2_{x\bar{y}}2_{xy}2_z$	$\bar{1}^\star, m_{xy}^\star, m_{x\bar{y}}^\star, m_z^\star$	$m_{x\bar{y}}^\star m_{xy}^\star m_z^\star$	A_u	=	1|0	0|0	3|0	3|0	0|3	0|9	0|12
$m_x m_y 2_z$	$\bar{1}^\star, m_z^\star, 2_x^\star, 2_y^\star$	$m_x m_y m_z^\star$	B_{1u}	=	0|0	1|0	1|0	5|0	0|3	0|9	0|12
$2_x m_y m_z$	$\bar{1}^\star, m_x^\star, 2_y^\star, 2_z^\star$	$m_x^\star m_y m_z$	B_{1u}	=	0|0	1|0	1|0	5|0	0|3	0|9	0|12
$m_x 2_y m_z$	$\bar{1}^\star, m_y^\star, 2_x^\star, 2_z^\star$	$m_x m_y^\star m_z$	B_{1u}	=	0|0	1|0	1|0	5|0	0|3	0|9	0|12
$m_{x\bar{y}} m_{xy} 2_z$	$\bar{1}^\star, m_z^\star, 2_{xy}^\star, 2_{x\bar{y}}^\star$	$m_{x\bar{y}} m_{xy} m_z^\star$	B_{1u}	=	0|0	1|0	1|0	5|0	0|3	0|9	0|12
4_z	$\bar{1}^\star, m_z^\star$	$4_z/m_z^\star$	A_u	=	1|0	1|0	2|0	4|0	0|4	0|7	0|10
4_z	$2_x^\star, 2_y^\star, 2_{xy}^\star, 2_{x\bar{y}}^\star$	$4_z 2_x^\star 2_{xy}^\star$	A_2	≠	0|1	1|0	0|2	3|1	3|1	1|6	3|7
4_z	$m_x^\star, m_y^\star, m_{xy}^\star, m_{x\bar{y}}^\star$	$4_z m_x^\star m_{xy}^\star$	A_2	≠	1|0	0|1	2|0	1|3	3|1	1|6	3|7
$\bar{4}_z$	$\bar{1}^\star, m_z^\star$	$4_z^\star/m_z^\star$	B_u	=	0|0	0|0	2|0	4|0	0|4	0|7	0|10
$\bar{4}_z$	$m_{xy}^\star, m_{x\bar{y}}^\star, 2_x^\star, 2_y^\star$	$\bar{4}_z 2_x^\star m_{xy}^\star$	A_2	≠	0|0	0|0	1|1	2|2	3|1	1|6	3|7
$\bar{4}_z$	$m_x^\star, m_y^\star, 2_{xy}^\star, 2_{x\bar{y}}^\star$	$\bar{4}_z m_x^\star 2_{xy}^\star$	A_2	≠	0|0	0|0	1|1	2|2	3|1	1|6	3|7
$4_z/m_z$	$m_x^\star, m_y^\star, m_{xy}^\star, m_{x\bar{y}}^\star, 2_x^\star, 2_y^\star, 2_{xy}^\star, 2_{x\bar{y}}^\star$	$4_z/m_z m_x^\star m_{xy}^\star$	A_{2g}	≠	0|0	0|0	0|0	0|0	3|1	1|6	3|7
$4_z 2_x 2_{xy}$	$\bar{1}^\star, m_z^\star, m_x^\star, m_y^\star, m_{xy}^\star, m_{x\bar{y}}^\star$	$4_z/m_z^\star m_x^\star m_{xy}^\star$	A_{1u}	=	1|0	0|0	2|0	1|0	0|1	0|6	0|7
$4_z m_x m_{xy}$	$\bar{1}^\star, m_z^\star, 2_x^\star, 2_y^\star, 2_{xy}^\star, 2_{x\bar{y}}^\star$	$4_z/m_z^\star m_x m_{xy}$	A_{2u}	=	0|0	1|0	0|0	3|0	0|1	0|6	0|7
$\bar{4}_z 2_x m_{xy}$	$\bar{1}^\star, m_z^\star, m_x^\star, m_y^\star, 2_{xy}^\star, 2_{x\bar{y}}^\star$	$4_z^\star/m_z^\star m_x^\star m_{xy}$	B_{1u}	=	0|0	0|0	1|0	2|0	0|1	0|6	0|7
$\bar{4}_z m_x 2_{xy}$	$\bar{1}^\star, m_z^\star, m_{xy}^\star, m_{x\bar{y}}^\star, 2_x^\star, 2_y^\star$	$4_z^\star/m_z^\star m_x m_{xy}^\star$	B_{1u}	=	0|0	0|0	1|0	2|0	0|1	0|6	0|7
3_v‡	$\bar{1}^\star$	$\bar{3}_v^\star$	A_u	=	1|0	1|0	2|0	6|0	0|6	0|7	0|12
3_z	$2_x^\star, 2_{x'}^\star, 2_{x''}^\star$	$3_z 2_x^\star$	A_2	≠	0|1	1|0	0|2	4|2	4|2	1|6	4|8
3_z	$2_y^\star, 2_{y'}^\star, 2_{y''}^\star$	$3_z 2_y^\star$	A_2	≠	0|1	1|0	0|2	4|2	4|2	1|6	4|8
3_p	$2_{x\bar{y}}^\star, 2_{y\bar{z}}^\star, 2_{z\bar{x}}^\star$	$3_p 2_{x\bar{y}}^\star$	A_2	≠	0|1	1|0	0|2	4|2	4|2	1|6	4|8
3_z	$m_x^\star, m_{x'}^\star, m_{x''}^\star$	$3_z m_x^\star$	A_2	≠	1|0	0|1	2|0	2|4	4|2	1|6	4|8
3_z	$m_y^\star, m_{y'}^\star, m_{y''}^\star$	$3_z m_y^\star$	A_2	≠	1|0	0|1	2|0	2|4	4|2	1|6	4|8
3_p	$m_{x\bar{y}}^\star, m_{y\bar{z}}^\star, m_{z\bar{x}}^\star$	$3_p m_x^\star$	A_2	≠	1|0	0|1	2|0	2|4	4|2	1|6	4|8
3_z	$2_z^\star$	$6_z^\star$	B	≠	0|1	0|1	0|2	2|4	2|4	2|5	4|8
3_z	$m_z^\star$	$\bar{6}_z^\star$	A''	≠	1|0	1|0	2|0	4|2	2|4	2|5	4|8
$\bar{3}_z$	$m_x^\star, m_{x'}^\star, m_{x''}^\star, 2_x^\star, 2_{x'}^\star, 2_{x''}^\star$	$\bar{3}_z m_x^\star$	A_{2g}	≠	0|0	0|0	0|0	0|0	4|2	1|6	4|8
$\bar{3}_z$	$m_y^\star, m_{y'}^\star, m_{y''}^\star, 2_y^\star, 2_{y'}^\star, 2_{y''}^\star$	$\bar{3}_z m_y^\star$	A_{2g}	≠	0|0	0|0	0|0	0|0	4|2	1|6	4|8
$\bar{3}_p$	$m_{x\bar{y}}^\star, m_{y\bar{z}}^\star, m_{z\bar{x}}^\star, 2_{x\bar{y}}^\star, 2_{y\bar{z}}^\star, 2_{z\bar{x}}^\star$	$\bar{3}_p m_x^\star$	A_{2g}	≠	0|0	0|0	0|0	0|0	4|2	1|6	4|8
$\bar{3}_z$	$m_z^\star, 2_z^\star$	$6_z^\star/m_z$	B_g	≠	0|0	0|0	0|0	0|0	2|4	2|5	4|8
$3_z 2_x$	$\bar{1}^\star, m_x^\star, m_{x'}^\star, m_{x''}^\star$	$\bar{3}_z m_x^\star$	A_{1u}	=	1|0	0|0	2|0	2|0	0|2	0|6	0|8
$3_z 2_y$	$\bar{1}^\star, m_y^\star, m_{y'}^\star, m_{y''}^\star$	$\bar{3}_z m_y^\star$	A_{1u}	=	1|0	0|0	2|0	2|0	0|2	0|6	0|8
$3_z 2_x$	$2_z^\star, 2_y^\star, 2_{y'}^\star, 2_{y''}^\star$	$6_z^\star 2_x 2_y^\star$	B_1	≠	0|1	0|0	0|2	1|1	1|1	1|5	2|6
$3_z 2_y$	$2_z^\star, 2_x^\star, 2_{x'}^\star, 2_{x''}^\star$	$6_z^\star 2_x^\star 2_y$	B_1	≠	0|1	0|0	0|2	1|1	1|1	1|5	2|6
$3_p 2_{x\bar{y}}$	$\bar{1}^\star, m_{x\bar{y}}^\star, m_{y\bar{z}}^\star, m_{z\bar{x}}^\star$	$\bar{3}_p m_x^\star$	A_{1u}	=	1|0	0|0	2|0	2|0	0|2	0|6	0|8
$3_z 2_x$	$m_z^\star, m_y^\star, m_{y'}^\star, m_{y''}^\star$	$\bar{6}_z^\star 2_x m_y^\star$	A_1''	≠	1|0	0|0	2|0	1|1	1|1	1|5	2|6
$3_z 2_y$	$m_z^\star, m_x^\star, m_{x'}^\star, m_{x''}^\star$	$\bar{6}_z^\star m_x 2_y^\star$	A_1''	≠	1|0	0|0	2|0	1|1	1|1	1|5	2|6
$3_p m_{x\bar{y}}$	$\bar{1}^\star, 2_{x\bar{y}}^\star, 2_{y\bar{z}}^\star, 2_{z\bar{x}}^\star$	$\bar{3}_p^\star m_x$	A_{2u}	=	0|0	1|0	0|0	4|0	0|2	0|6	0|8
$3_z m_x$	$\bar{1}^\star, 2_x^\star, 2_{x'}^\star, 2_{x''}^\star$	$\bar{3}_z^\star m_x$	A_{2u}	=	0|0	1|0	0|0	4|0	0|2	0|6	0|8
$3_z m_y$	$\bar{1}^\star, 2_y^\star, 2_{y'}^\star, 2_{y''}^\star$	$\bar{3}_z^\star m_y$	A_{2u}	=	0|0	1|0	0|0	4|0	0|2	0|6	0|8
$3_z m_x$	$2_z^\star, m_{y}^\star, m_{y'}^\star, m_{y''}^\star$	$6_z^\star m_x m_y^\star$	B_2	≠	0|0	0|1	0|0	1|3	1|1	1|5	2|6
$3_z m_y$	$m_x^\star, m_{x'}^\star, m_{x''}^\star$	$6_z^\star m_x^\star m_y$	B_2	≠	0|0	0|1	0|0	1|3	1|1	1|5	2|6
$3_z m_x$	$m_z^\star, 2_z^\star, 2_y^\star, 2_{y''}^\star$	$\bar{6}_z^\star m_x 2_y^\star$	A_2''	≠	0|0	1|0	0|0	3|1	1|1	1|5	2|6
$3_z m_y$	$m_z^\star, 2_z^\star, 2_x^\star, 2_{x''}^\star$	$\bar{6}_z^\star 2_x^\star m_y$	A_2''	≠	0|0	1|0	0|0	3|1	1|1	1|5	2|6
$\bar{3}_z m_x$	$m_z^\star, m_y^\star, m_{y'}^\star, m_{y''}^\star$	$6_z^\star/m_z m_x m_y^\star$	B_{1g}	≠	0|0	0|0	0|0	0|0	1|1	1|5	2|6
$\bar{3}_z m_y$	$m_z^\star, m_x^\star, m_{x'}^\star, m_{x''}^\star$	$6_z^\star/m_z m_x^\star m_y$	B_{1g}	≠	0|0	0|0	0|0	0|0	1|1	1|5	2|6
6_z	$\bar{1}^\star, m_z^\star$	$6_z/m_z^\star$	A_u	=	1|0	1|0	2|0	4|0	0|4	0|5	0|8
6_z	$2_x^\star, 2_{x'}^\star, 2_{x''}^\star, 2_y^\star, 2_{y'}^\star, 2_{y''}^\star$	$6_z 2_x^\star 2_y^\star$	A_2	≠	0|1	1|0	0|2	3|1	3|1	0|5	2|6
6_z	$m_x^\star, m_{x'}^\star, m_{x''}^\star, m_y^\star, m_{y'}^\star, m_{y''}^\star$	$6_z m_x^\star m_y^\star$	A_2	≠	1|0	0|1	2|0	1|3	3|1	0|5	2|6
$\bar{6}_z$	$\bar{1}^\star, 2_z^\star$	$6_z^\star/m_z$	B_u	=	0|0	0|0	0|0	2|0	0|4	0|5	0|8
$\bar{6}_z$	$m_x^\star, m_{x'}^\star, m_{x''}^\star, 2_y^\star, 2_{y'}^\star, 2_{y''}^\star$	$\bar{6}_z m_x^\star 2_y$	A_2'	≠	0|0	0|0	0|0	1|1	3|1	0|5	2|6
$\bar{6}_z$	$m_y^\star, m_{y'}^\star, m_{y''}^\star, 2_x^\star, 2_{x'}^\star, 2_{x''}^\star$	$\bar{6}_z 2_x^\star m_y$	A_2'	≠	0|0	0|0	0|0	1|1	3|1	0|5	2|6

† $u = z, x(x', x''), y(y', y''), xy(x\bar{y}, zx, z\bar{x}, yz, y\bar{z})$. ‡ $v = z, p(q, r, s)$.

Table 3.4.3.4 (*cont.*)

F_1	$g^\star_{1j}$	$K^\star_{1j} = J^\star_{1j}$	Γ_α	Diffraction intensities	ϵ	P_i	g_μ	$d_{i\mu}$	$A_{i\mu}$	$s_{\mu\nu}$	$Q_{ij\mu}$
$6_z/m_z$	$m^\star_x, m^\star_{x'}, m^\star_{x''}, m^\star_y, m^\star_{y'}, m^\star_{y''}, 2^\star_x, 2^\star_{x'}, 2^\star_{x''}, 2^\star_y, 2^\star_{y'}, 2^\star_{y''}$	$6_z/m_z m^\star_x m^\star_y$	A_{2g}	$\neq$	$0|0$	$0|0$	$0|0$	$0|0$	$3|1$	$0|5$	$2|6$
$6_z 2_x 2_y$	$\bar1^\star, m^\star_z, m^\star_x, m^\star_{x'}, m^\star_{x''}, m^\star_y, m^\star_{y'}, m^\star_{y''}$	$6_z/m^\star_z m^\star_x m^\star_y$	A_{1u}	$=$	$1|0$	$0|0$	$2|0$	$1|0$	$0|1$	$0|5$	$0|6$
$6_z m_x m_y$	$\bar1^\star, m^\star_z, 2^\star_x, 2^\star_{x'}, 2^\star_{x''}, 2^\star_y, 2^\star_{y'}, 2^\star_{y''}$	$6_z/m^\star_z m_x m_y$	A_{2u}	$=$	$0|0$	$1|0$	$0|0$	$3|0$	$0|1$	$0|5$	$0|6$
$\bar6_z 2_x m_y$	$\bar1^\star, 2^\star_z, m^\star_x, m^\star_{x'}, m^\star_{x''}, 2^\star_y, 2^\star_{y'}, 2^\star_{y''}$	$6^\star_z/m_z m^\star_x m_y$	B_{2u}	$=$	$0|0$	$0|0$	$0|0$	$1|0$	$0|1$	$0|5$	$0|6$
$\bar6_z m_x 2_y$	$\bar1^\star, 2^\star_z, m^\star_y, m^\star_{y'}, m^\star_{y''}, 2^\star_x, 2^\star_{x'}, 2^\star_{x''}$	$6^\star_z/m_z m_x m^\star_y$	B_{2u}	$=$	$0|0$	$0|0$	$0|0$	$1|0$	$0|1$	$0|5$	$0|6$
23	$\bar1^\star, m^\star_x, m^\star_y, m^\star_z$	$m^\star\bar3$	A_u	$=$	$1|0$	$0|0$	$1|0$	$1|0$	$0|1$	$0|3$	$0|4$
23	$2^\star_{xy}, 2^\star_{yz}, 2^\star_{zx}, 2^\star_{x\bar y}, 2^\star_{y\bar z}, 2^\star_{z\bar x}$	$4^\star 32^\star$	A_2	$\neq$	$0|1$	$0|0$	$0|1$	$1|0$	$1|0$	$0|3$	$1|3$
23	$m^\star_{xy}, m^\star_{yz}, m^\star_{zx}, m^\star_{x\bar y}, m^\star_{y\bar z}, m^\star_{z\bar x}$	$\bar4^\star 3 m^\star$	A_2	$\neq$	$1|0$	$0|0$	$1|0$	$0|1$	$1|0$	$0|3$	$1|3$
$m\bar3$	$m^\star_{xy}, m^\star_{yz}, m^\star_{zx}, m^\star_{x\bar y}, m^\star_{y\bar z}, m^\star_{z\bar x}, 2^\star_{xy}, 2^\star_{yz}, 2^\star_{zx}, 2^\star_{x\bar y}, 2^\star_{y\bar z}, 2^\star_{z\bar x}$	$m\bar3 m^\star$	A_{2g}	$\neq$	$0|0$	$0|0$	$0|0$	$0|0$	$1|0$	$0|3$	$1|3$
432	$\bar1^\star, m^\star_x, m^\star_y, m^\star_z, m^\star_{xy}, m^\star_{yz}, m^\star_{zx}, m^\star_{x\bar y}, m^\star_{y\bar z}, m^\star_{z\bar x}$	$m^\star\bar3m^\star$	A_{1u}	$=$	$1|0$	$0|0$	$1|0$	$0|0$	$0|0$	$0|3$	$0|3$
$\bar43m$	$\bar1^\star, m^\star_x, m^\star_y, m^\star_z, 2^\star_{xy}, 2^\star_{yz}, 2^\star_{zx}, 2^\star_{x\bar y}, 2^\star_{y\bar z}, 2^\star_{z\bar x}$	$m^\star\bar3m$	A_{2u}	$=$	$0|0$	$0|0$	$0|0$	$1|0$	$0|0$	$0|3$	$0|3$

non-ferroelastic twins with domains containing $\mathbf{S}_1$ *and* $\mathbf{S}_j$ (see Section 3.4.3.1).

The second part of the table concerns the *distinction and switching* of domain states of the non-ferroelastic domain pair $(\mathbf{S}_1, \mathbf{S}_j) = (\mathbf{S}_1, g^\star_{1j}\mathbf{S}_1)$.

Γ_α: irreducible representation of K_{1j} that defines the transformation properties of the principal tensor parameters of the symmetry descent $K_{1j} \supset F_1$ and thus specifies the components of principal tensor parameters that are given explicitly in Table 3.1.3.1, in the software *GI⋆KoBo*-1 and in Kopský (2001), where one replaces G by K_{1j}.

Diffraction intensities: the entries in this column characterize the differences of diffraction intensities from two domain states of the domain pair:

$=$ signifies that the twinning operations belong to the Laue class of F_1. Then the reflection intensities per unit volume are the same for both domain states if anomalous scattering is zero, *i.e.* if Friedel's law is valid. For nonzero anomalous scattering, the intensities from the two domain states differ, but when the partial volumes of both states are equal the diffraction pattern is centrosymmetric;

$\neq$ signifies that the twinning operations do not belong to the Laue class of F_1. Then the reflection intesities per unit volume of the two domain states are different [for more details, see Chapter 3.3; Catti & Ferraris (1976); Koch (1999)].

ϵ, P_i, g_μ,..., $Q_{ij\mu}$: components (in matrix notation) of important *property tensors* that are specified in Table 3.4.3.5. The same symbol may represent several property tensors (given in the same row of Table 3.4.3.5) of the same rank and intrinsic symmetry. Bold-face symbols signify polar tensors. For each type of property tensor two numbers $a|c$ are given; number a in front of the vertical bar | is the *number of independent covariant components* (in most cases identical with Cartesian components) that have the *same absolute value but different sign in domain states* $\mathbf{S}_1$ and $\mathbf{S}_j$. The number c after the vertical bar | gives the *number of independent nonzero tensor parameters that have equal values in both domain states* of the domain pair $(\mathbf{S}_1, \mathbf{S}_j)$. These tensor components are already nonzero in the parent phase.

Table 3.4.3.5. *Property tensors and switching fields*

$i = 1, 2, 3$; $\mu, \nu = 1, 2, \ldots, 6$.

Symbol	Property tensor	Symbol	Property tensor	Switching fields
ϵ	Enantiomorphism		Chirality	
P_i	Polarization	p_i	Pyroelectricity	**E**
ε_{ij}	Permittivity			**EE**
g_μ	Optical activity			
$d_{i\mu}$	Piezoelectricity	r_{ijk}	Electro-optics	**Eu**
$A_{i\mu}$	Electrogyration			
$s_{\mu\nu}$	Elastic compliances			**uu**
$Q_{ij\mu}$	Electrostriction	$\pi_{ij\mu}$	Piezo-optics	**EEu**

The principal tensor parameters are one-dimensional and have the same absolute value but opposite sign in $\mathbf{S}_1$ and $\mathbf{S}_j = g^\star_{1j}\mathbf{S}_1$. Principal tensor parameters for symmetry descents $K_{1j} \supset F_1$ and the associated Γ_α of all non-ferroelastic domain pairs can be found for property tensors of lower rank in Table 3.1.3.1 and for all tensors appearing in Table 3.4.3.4 in the software *GI⋆KoBo*-1 and in Kopský (2001), where one replaces G by K_{1j}.

When $a \neq 0$ for a polar tensor (in bold-face components), then *switching fields* exist in the combination given in the last column of Table 3.4.3.5. Components of these fields can be determined from the explicit form of corresponding principal tensor parameters expressed in Cartesian components.

Table 3.4.3.5 lists important property tensors up to fourth rank. Property tensor components that appear in the column headings of Table 3.4.3.4 are given in the first column, where bold face is used for the polar tensors significant for specifying the switching fields appearing in schematic form in the last column. In the third and fourth columns, those propery tensors appear for which hold all the results presented in Table 3.4.3.4 for the symbols given in the first column of Table 3.4.3.5.

We turn attention to Section 3.4.5 (Glossary), which describes the difference between the notation of tensor components in matrix notation given in Chapter 1.1 and those used in the software *GI⋆KoBo*-1 and in Kopský (2001).

The numbers a in front of the vertical bar | in Table 3.4.3.4 provide global information about the tensor distinction of two domain states and enables one to classify domain pairs. Thus, for example, the first number a in column P_i gives the number of nonzero components of the spontaneous polarization that differ in sign in both domain states; if $a \neq 0$, this domain pair can be classified as a *ferroelectric domain pair*.

Similarly, the first number a in column g_μ determines the number of independent components of the tensor of optical activity that have opposite sign in domain states $\mathbf{S}_1$ and $\mathbf{S}_j$; if $a \neq 0$, the two domain states in the pair can be distinguished by optical activity. Such a domain pair can be called a *gyrotropic domain pair*. As in Table 3.4.3.1 for the ferroelectric (ferroelastic) domain pairs, we can define a *gyrotropic phase* as a ferroic phase with gyrotropic domain pairs. The corresponding phase transition to a gyrotropic phase is called a *gyrotropic phase transition* (Koňák *et al.*, 1978; Wadhawan, 2000). If it is possible to switch gyrotropic domain states by an external field, the phase is called a *ferrogyrotropic phase* (Wadhawan, 2000). Further division into full and partial subclasses is possible.

One can also define *piezoelectric (electro-optic) domain pairs*, *electrostrictive (elasto-optic) domain pairs* and corresponding phases and transitions.

As we have already stated, domain states in a domain pair $(\mathbf{S}_1, \mathbf{S}_j)$ differ in principal tensor parameters of the transition $K_{1j} \supset F_1$. These principal tensor parameters are Cartesian tensor
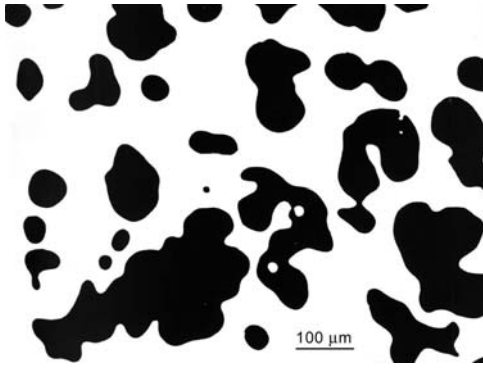
Fig. 3.4.3.3. Domain structure in lead germanate observed using a polarized-light microscope. Visualization based on the opposite sign of the optical activity coefficient in the two domain states. Courtesy of Vl. Shur, Ural State University, Ekaterinburg.

components or their linear combinations that transform according to an irreducible representation Γ_α specifying the primary order parameter of the transition $K_{1j} \supset F_1$ (see Section 3.1.3). Owing to a special form of K_{1j} expressed by equation (3.4.3.42), this representation is a real one-dimensional irreducible representation of K_{1j}. Such a representation associates $+1$ with operations of F_1 and -1 with operations from the left coset $g^\star_{1j}$. This means that the principal tensor parameters are one-dimensional and have the same absolute value but opposite sign in $\mathbf{S}_1$ and $\mathbf{S}_j = g^\star_{1j}\mathbf{S}_1$. Principal tensor parameters for symmetry descents $K_{1j} \supset F_1$ and associated Γ_α's of all non-ferroelastic domain pairs can be found for property tensors of lower rank in Table 3.1.3.1 and for all tensors appearing in Table 3.4.3.5 in the software $GI\star KoBo$-1 and in Kopský (2001).

These specific properties of non-ferroelastic domain pairs allow one to formulate simple rules for tensor distinction that do not use principal tensor parameters and that are applicable for property tensors of lower rank.

(i) Symmetry descents $K_{1j} \supset F_1$ of non-ferroelastic domain pairs for lower-rank property tensors lead only to the appearance of independent Cartesian morphic tensor components and not to the breaking of relations between these components. These morphic Cartesian tensor components can be found by comparing matrices of property tensors in the twinning group K_{1j} and the low-symmetry group F_1 as those components that appear in F_1 but are zero in K_{1j}.

(ii) As follows from Table 3.4.3.4, one can always find a twinning operation that is either inversion, or a twofold axis or a mirror plane with a prominent crystallographic orientation. By applying the method of direct inspection (see Section 1.1.4.6.3), one can in most cases easily find morphic Cartesian components in the second domain state of the domain pair considered and prove that they differ only in sign.

Example 3.4.3.4. *Tensor distinction of domains and switching in lead germanate.* Lead germanate ($Pb_5Ge_3O_{11}$) undergoes a phase transition with symmetry descent $G = 6 \supset 3 = F_1$ for which we find in Table 3.4.2.7, column K_{1j}, just one twinning group $K_{1j} = \bar{6}^\star$, i.e. $K^\star_{1j} = G$. This means that there is only one G-orbit of domain pairs. Since Fam3 = Fam$\bar{6}$ [see Table 3.4.2.2 and equation (3.4.3.40)] this orbit comprises non-ferroelastic domain pairs. In Table 3.4.3.4, we find for $F_1 = 3$ and $F^\star_{1j} = \bar{6}$ that the two domain states differ in some components of all property tensors listed in this table. The first polar tensor is the spontaneous polarization (the pair is ferroelectric) with one component ($a = 1$) that has opposite sign in the two domain states. In Table 3.1.3.1, we find for $G(= K_{1j}) = 6$ and $F_1 = 3$ that this component is $P_3 = P_z$. From Table 3.4.3.1, it follows that the state shift is electrically first order with switching field $\mathbf{E} = (0, 0, E_z)$.

The first optical tensor, which could enable the visualization of the domain states, is the optical activity g_μ with two independent components which have opposite sign in the two domain states. In the software $GI\star KoBo$-1, path: *Subgroups\View\Domains* or in Kopský (2001) we find these components: g_3, $g_1 + g_2$. Shur *et al.* (1989) have visualized in this way the domain structure of lead germanate with excellent black and white contrast (see Fig. 3.4.3.3). Other examples are given in Shuvalov & Ivanov (1964) and especially in Koňák *et al.* (1978).

Table 3.4.3.4 can be used readily for twinning by merohedry [see Chapter 3.3 and *e.g.* Cahn (1954); Koch (1999)], where it enables an easy determination of the tensor distinction of twin components and the specification of external fields for possible switching and detwinning.

Example 3.4.3.5. *Tensor distinction and switching of Dauphiné twins in quartz.* Quartz undergoes a phase transition from $G = 6_z2_x2_y$ to $F_1 = 3_z2_x$. Using the same procedure as in the previous example, we come to following conclusions: There are only two domain states $\mathbf{S}_1$, $\mathbf{S}_2$ and the twinning group, expressing the twin law, is equal to the high-symmetry group $K^\star_{12} = 6_zx2_y$. In Table 3.4.3.4, we find that these two states differ in one independent component of the piezoelectric tensor and in one elastic compliance component. Comparison of the matrices for $6_z2_x2_y$ and 3_z2_x (see Sections 1.1.4.10.3 and 1.1.4.10.4) yields the following morphic tensor components in the first domain state $\mathbf{S}_1$: $d^{(1)}_{11} = -d^{(1)}_{12} = -2d^{(1)}_{26}$ and $s^{(1)}_{14} = -s^{(1)}_{24} = 2s^{(1)}_{56}$. According to the rule given above, the values of morphic components in the second domain state $\mathbf{S}_2$ are $d^{(2)}_{11} = -d^{(1)}_{11} = -d^{(2)}_{12} = d^{(1)}_{12} = -2d^{(2)}_{26} = 2d^{(1)}_{26}$ and $s^{(2)}_{14} = -s^{(1)}_{14} = -s^{(2)}_{24} = s^{(1)}_{24} = 2s^{(2)}_{56} = -2s^{(1)}_{56}$ [see Section 3.4.5 (Glossary)]. These results show that there is an elastic state shift of second order and an electromechanical state shift of second order. Nonzero components $d_{14} = -d_{25}$ in $6_z2_x2_y$ are the same in both domain states. Similarly, one can find five independent components of the tensor $s_{\mu\nu}$ that are nonzero in $6_z2_x2_y$ and equal in both domain states. For the piezo-optic tensor $\pi_{\mu\nu}$, one can proceed in a similar way. Aizu (1973) has used the ferrobielastic character of the domain pairs for visualizing domains and realizing switching in quartz. Other methods for switching and visualizing domains in quartz are known (see *e.g.* Bertagnolli *et al.*, 1978, 1979).

3.4.3.6. *Ferroelastic domain pairs*

A *ferroelastic domain pair* consists of two domain states that have different spontaneous strain. A domain pair $(\mathbf{S}_1, \mathbf{S}_j)$ is a ferroelastic domain pair if the crystal family of its twinning group K_{1j} differs from the crystal family of the symmetry group F_1 of domain state $\mathbf{S}_1$,

$$\mathrm{Fam}K_{1j} \neq \mathrm{Fam}F_1. \qquad (3.4.3.43)$$

Before treating compatible domain walls and disorientations, we explain the basic concept of spontaneous strain.

3.4.3.6.1. *Spontaneous strain*

A *strain* describes a *change* of crystal shape (in a macroscopic description) or a change of the unit cell (in a microscopic description) under the influence of mechanical stress, temperature or electric field. If the relative changes are small, they can be described by a second-rank symmetric tensor $\mathbf{u}$ called the *Lagrangian strain*. The values of the strain components u_{ik}, $i, k = 1, 2, 3$ (or in matrix notation u_μ, $\mu = 1, \ldots, 6$) can be calculated from the 'undeformed' unit-cell parameters before deformation and 'deformed' unit-cell parameters after deformation (see Schlenker *et al.*, 1978; Salje, 1990; Carpenter *et al.*, 1998).
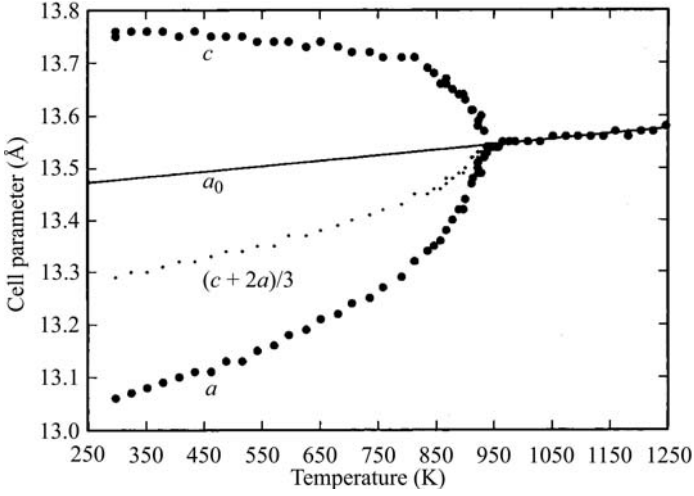
Fig. 3.4.3.4. Temperature dependence of lattice parameters in leucite. Courtesy of E. K. H Salje, University of Cambridge.

A *spontaneous strain* describes the change of an 'undeformed' unit cell of the high-symmetry phase into a 'deformed' unit cell of the low-symmetry phase. To exclude changes connected with thermal expansion, one demands that the parameters of the undeformed unit cell are those that the high-symmetry phase would have at the temperature at which parameters of the low-symmetry phase are measured. To determine these parameters directly is not possible, since the parameters of the high-symmetry phase can be measured only in the high-symmetry phase. One uses, therefore, different procedures in order to estimate values for the high-symmetry parameters under the external conditions to which the measured values of the low-symmetry phase refer (see *e.g.* Salje, 1990; Carpenter *et al.*, 1998). Three main strategies are illustrated using the example of leucite (see Fig. 3.4.3.4):

(i) The lattice parameters of the high-symmetry phase are extrapolated from values measured in the high-symmetry phase (a straight line a_0 in Fig. 3.4.3.4). This is a preferred approach.

(ii) For certain symmetry descents, it is possible to approximate the high-symmetry parameters in the low-symmetry phase by average values of the lattice parameters in the low-symmetry phase. Thus for example in cubic $\rightarrow$ tetragonal transitions one can take for the cubic lattice parameter $a_0 = (2a + c)/3$ (the dotted curve in Fig. 3.4.3.4), for cubic $\rightarrow$ orthorhombic transitions one may assume $a_0 = (abc)^{1/3}$, where a, b, c are the lattice parameters of the low-symmetry phase. Errors are introduced if there is a significant volume strain, as in leucite.

(iii) Thermal expansion is neglected and for the high-symmetry parameters in the low-symmetry phase one takes the lattice parameters measured in the high-symmetry phase as close as possible to the transition. This simplest method gives better results than average values in leucite, but in general may lead to significant errors.

Spontaneous strain has been examined in detail in many ferroic crystals by Carpenter *et al.* (1998).

Spontaneous strain can be divided into two parts: one that is different in all ferroelastic domain states and the other that is same in all ferroelastic domain states. This division can be achieved by introducing a *modified strain tensor* (Aizu, 1970*b*), also called a *relative spontaneous strain* (Wadhawan, 2000):

$$\mathbf{u}^{(i)}_{(s)} = \mathbf{u}^{(i)} - \mathbf{u}^{(av)}_{(s)}, \qquad (3.4.3.44)$$

where $\mathbf{u}^{(i)}_{(s)}$ is the matrix of relative (modified) spontaneous strain in the ferroelastic domain state $\mathbf{R}_i$, $\mathbf{u}^{(i)}$ is the matrix of an 'absolute' spontaneous strain in the same ferroelastic domain state $\mathbf{R}_i$ and $\mathbf{u}^{(av)}_{(s)}$ is the matrix of an *average spontaneous strain*

that is equal to the sum of the matrices of absolute spontaneous strains over all n_a ferroelastic domain states,

$$\mathbf{u}^{(av)} = \frac{1}{n_a} \sum_{j=1}^{n_a} \mathbf{u}^{(j)}. \qquad (3.4.3.45)$$

The relative spontaneous strain $\mathbf{b}^{(i)}_{(s)}$ is a *symmetry-breaking strain* that transforms according to a non-identity representation of the parent group G, whereas the average spontaneous strain is a *non-symmetry breaking strain* that transforms as the identity representation of G.

Example 3.4.3.6. We illustrate these concepts with the example of symmetry descent $4_z/m_z m_x m_{xy} \supset 2_x m_y m_z$ with two ferroelastic domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ (see Fig. 3.4.2.2). The absolute spontaneous strain in the first ferroelastic domain state $\mathbf{R}_1$ is

$$\mathbf{u}^{(1)} = \begin{pmatrix} \frac{a-a_0}{a_0} & 0 & 0 \\ 0 & \frac{b-a_0}{a_0} & 0 \\ 0 & 0 & \frac{c-c_0}{c_0} \end{pmatrix} = \begin{pmatrix} u_{11} & 0 & 0 \\ 0 & u_{22} & 0 \\ 0 & 0 & u_{33} \end{pmatrix}, \qquad (3.4.3.46)$$

where a, b, c and a_0, b_0, c_0 are the lattice parameters of the orthorhombic and tetragonal phases, respectively.

The spontaneous strain $\mathbf{u}^{(2)}$ in domain state $\mathbf{R}_2$ is obtained by applying to $\mathbf{u}^{(1)}$ any switching operation that transforms $\mathbf{R}_1$ into $\mathbf{R}_2$ (see Table 3.4.2.1),

$$\mathbf{u}^{(2)} = \begin{pmatrix} u_{22} & 0 & 0 \\ 0 & u_{11} & 0 \\ 0 & 0 & u_{33} \end{pmatrix}. \qquad (3.4.3.47)$$

The average spontaneous strain is, according to equation (3.4.3.45),

$$\mathbf{u}^{(av)} = \frac{1}{2} \begin{pmatrix} u_{11} + u_{22} & 0 & 0 \\ 0 & u_{11} + u_{22} & 0 \\ 0 & 0 & u_{33} + u_{33} \end{pmatrix}. \qquad (3.4.3.48)$$

This deformation is invariant under any operation of G.

The relative spontaneous strains in ferroelastic domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ are, according to equation (3.4.3.44),

$$\mathbf{u}^{(1)}_{(s)} = \mathbf{u}^{(1)} - \mathbf{u}^{(av)} = \begin{pmatrix} \frac{1}{2}(u_{11} - u_{22}) & 0 & 0 \\ 0 & -\frac{1}{2}(u_{11} - u_{22}) & 0 \\ 0 & 0 & 0 \end{pmatrix},$$
$$(3.4.3.49)$$

$$\mathbf{u}^{(2)}_{(s)} = \mathbf{u}^{(2)} - \mathbf{u}^{(av)} = \begin{pmatrix} -\frac{1}{2}(u_{11} - u_{22}) & 0 & 0 \\ 0 & \frac{1}{2}(u_{11} - u_{22}) & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$
$$(3.4.3.50)$$

Symmetry-breaking nonzero components of the relative spontaneous strain are identical, up to the factor $\frac{1}{2}$, with the secondary tensor parameters $\lambda^{(1)}_b$ and $\lambda^{(2)}_b$ of the transition $4_z/m_z m_x m_{xy} \supset 2_x m_y m_z$ with the stabilizer $I_{4_z/m_z m_x m_{xy}}(\mathbf{R}_1) = I_{4_z/m_z m_x m_{xy}}(\mathbf{R}_2) = m_x m_y m_z$. The non-symmetry-breaking component u_{33} does not appear in the relative spontaneous strain.

The form of relative spontaneous strains for all ferroelastic domain states of all full ferroelastic phases are listed in Aizu (1970*b*).

3.4.3.6.2. *Equally deformed planes of a ferroelastic domain pair*

We start with the example of a phase transition with the symmetry descent $G = 4_z/m_z m_x m_{xy} \supset 2_x m_y m_z$, which generates two ferroelastic single-domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ (see Fig. 3.4.2.2).
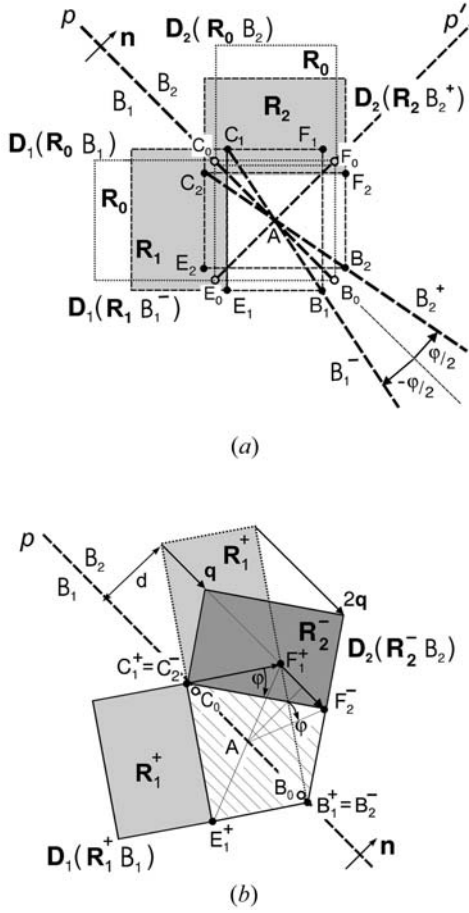
(a)

(b)

Fig. 3.4.3.5. Formation of a ferroelastic domain twin. (a) Formation of ferroelastic single-domain states $\mathbf{R}_1$, $\mathbf{R}_2$ from the parent phase $\mathbf{R}_0$; p and p' are two perpendicular planes of equal deformation. (b) Formation of a ferroelastic twin: (i) by rotating the single-domain states $\mathbf{S}_1$, $\mathbf{S}_2$ in (a) through an angle $\pm\frac{1}{2}\varphi$ about the domain-pair axis A ($\mathbf{R}_1^+$ and $\mathbf{R}_2^-$ are the resulting disoriented ferroelastic domain states); (ii) by a simple shear deformation with a shear angle (obliquity) φ.

An 'elementary cell' of the parent phase is represented in Fig. 3.4.3.5(a) by a square $B_0E_0C_0F_0$ and the corresponding domain state is denoted by $\mathbf{R}_0$.

In the ferroic phase, the square $B_0E_0C_0F_0$ can change either under spontaneous strain $\mathbf{u}^{(1)}$ into a spontaneously deformed rectangular cell $B_1E_1C_1F_1$ representing a domain state $\mathbf{R}_1$, or under a spontaneous strain $\mathbf{u}^{(2)}$ into rectangular $B_2E_2C_2F_2$ representing domain state $\mathbf{R}_2$. We shall use the letter $\mathbf{R}_0$ as a symbol of the parent phase and $\mathbf{R}_1$, $\mathbf{R}_2$ as symbols of two ferroelastic single-domain states.

Let us now choose in the parent phase a vector $\overrightarrow{AB_0}$. This vector changes into $\overrightarrow{AB_1}$ in ferroelastic domain state $\mathbf{R}_1$ and into $\overrightarrow{AB_2}$ in ferroelastic domain state $\mathbf{R}_1$. We see that the resulting vectors $\overrightarrow{AB_1}$ and $\overrightarrow{AB_2}$ have different direction but equal length: $|\overrightarrow{AB_1}| = |\overrightarrow{AB_2}|$. This consideration holds for any vector in the plane p, which can therefore be called an *equally deformed plane* (EDP). One can find that the perpendicular plane p' is also an equally deformed plane, but there is no other plane with this property.

The intersection of the two perpendicular equally deformed planes p and p' is a line called an *axis of the ferroelastic domain pair* $(\mathbf{R}_1, \mathbf{R}_2)$ (in Fig. 3.4.3.5 it is a line at A perpendicular to the paper). This axis is the only line in which any vector chosen in the parent phase exhibits equal deformation and has its direction unchanged in both single-domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ of a ferroelastic domain pair.

This consideration can be expressed analytically as follows (Fousek & Janovec, 1969; Sapriel, 1975). We choose in the parent phase a plane p and a unit vector $\mathbf{v}(x_1, x_2, x_3)$ in this plane. The changes of lengths of this vector in the two ferroelastic domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ are $u_{ik}^{(1)}x_ix_k$ and $u_{ik}^{(2)}x_ix_k$, respectively, where $u_{ik}^{(1)}$ and $u_{ik}^{(2)}$ are spontaneous strains in $\mathbf{R}_1$ and $\mathbf{R}_2$, respectively (see *e.g.* Nye, 1985). (We are using the Einstein summation convention: when a letter suffix occurs twice in the same term, summation with respect to that suffix is to be understood.) If these changes are equal, *i.e.* if

$$u_{ik}^{(1)}x_ix_k = u_{ik}^{(2)}x_ix_k, \qquad (3.4.3.51)$$

for any vector $\mathbf{v}(x_1, x_2, x_3)$ in the plane p this plane will be an equally deformed plane. If we introduce a *differential spontaneous strain*

$$\Delta u_{ik} \equiv u_{ik}^{(2)} - u_{ik}^{(1)}, \quad i, k = 1, 2, 3, \qquad (3.4.3.52)$$

the condition (3.4.3.51) can be rewritten as

$$\Delta u_{ik}x_ix_j = 0. \qquad (3.4.3.53)$$

This equation describes a cone with the apex at the origin. The cone degenerates into two planes if the determinant of the differential spontaneous strain tensor equals zero,

$$\det\Delta u_{ik} = 0. \qquad (3.4.3.54)$$

If this condition is satisfied, two solutions of (3.4.3.53) exist:

$$Ax_1 + Bx_2 + Cx_3 = 0, \quad A'x_1 + B'x_2 + C'x_3 = 0. \qquad (3.4.3.55)$$

These are equations of two planes p and p' passing through the origin. Their normal vectors are $\mathbf{n} = [ABC]$ and $\mathbf{n}' = [A'B'C']$. It can be shown that from the equation

$$\Delta u_{11} + \Delta u_{22} + \Delta u_{33} = 0, \qquad (3.4.3.56)$$

which holds for the trace of the matrix $\det\Delta u_{ik}$, it follows that these two planes are perpendicular:

$$AA' + BB' + CC' = 0. \qquad (3.4.3.57)$$

The intersection of these equally deformed planes (3.4.3.53) is the *axis of the ferroelastic domain pair* $(\mathbf{R}_1, \mathbf{R}_2)$.

Let us illustrate the application of these results to the domain pair $(\mathbf{R}_1, \mathbf{R}_2)$ depicted in Fig. 3.4.3.1(b) and discussed above. From equations (3.4.3.41) and (3.4.3.47), or (3.4.3.49) and (3.4.3.50) we find the only nonzero components of the difference strain tensor are

$$\Delta u_{11} = u_{22} - u_{11}, \quad \Delta u_{22} = u_{11} - u_{22}. \qquad (3.4.3.58)$$

Condition (3.4.3.54) is fulfilled and equation (3.4.3.53) is

$$\Delta u_{11}x_1^2 + \Delta u_{22}x_2^2 = (u_{22} - u_{11})x_1^2 + (u_{11} - u_{22})x_2^2 = 0. \qquad (3.4.3.59)$$

There are two solutions of this equation:

$$x_1 = x_2, \quad x_1 = -x_2. \qquad (3.4.3.60)$$

These two equally deformed planes p and p' have the normal vectors $\mathbf{n} = [\bar{1}10]$ and $\mathbf{n} = [110]$. The axis of this domain pair is directed along [001].

Equally deformed planes in our example have the same orientations as have the mirror planes $m_{\bar{x}y}$ and m_{xy} lost at the transition $4_z/m_zm_xm_{xy} \supset m_xm_ym_z$. From Fig. 3.4.3.5(a) it is clear why: reflection $m_{\bar{x}y}$, which is a transposing operation of the domain pair $(\underline{\mathbf{R}}_1, \mathbf{R}_2)$, ensures that the vectors $\overrightarrow{AB_1}$ and $\overrightarrow{AB_2}$ arising from $\overrightarrow{AB_0}$ have equal length. A similar conclusion holds for a 180° rotation and a plane perpendicular to the corresponding twofold axis. Thus we come to two useful rules:

Any reflection through a plane that is a transposing operation of a ferroelastic domain pair ensures the existence of two planes of

equal deformation: one is parallel to the corresponding mirror plane and the other one is perpendicular to this mirror plane.

Any 180° rotation that is a transposing operation of a ferroelastic domain pair ensures the existence of two equally deformed planes: one is perpendicular to the corresponding twofold axis and the other one is parallel to this axis.

A reflection in a plane or a 180° rotation generates at least one equally deformed plane with a fixed prominent *crystallographic orientation* independent of the magnitude of the spontaneous strain; the other perpendicular equally deformed plane may have a *non-crystallographic orientation* which depends on the spontaneous strain and changes with temperature. If between switching operations there are two reflections with corresponding perpendicular mirror planes, or two 180° rotations with corresponding perpendicular twofold axes, or a reflection and a 180° rotation with a corresponding twofold axis parallel to the mirror, then both perpendicular equally deformed planes have fixed crystallographic orientations. If there are no switching operations of the second order, then both perpendicular equally deformed planes may have non-crystallographic orientations, or equally deformed planes may not exist at all.

Equally deformed planes in ferroelastic–ferroelectric phases have been tabulated by Fousek (1971). Sapriel (1975) lists equations (3.4.3.55) of equally deformed planes for all ferroelastic phases. Table 3.4.3.6 contains the orientation of equally deformed planes (with further information about the walls) for representative domain pairs of all orbits of ferroelastic domain pairs. Table 3.4.3.7 lists representative domain pairs of all ferroelastic orbits for which no compatible walls exist.

3.4.3.6.3. *Disoriented domain states, ferroelastic domain twins and their twin laws*

To examine another possible way of forming a ferroelastic domain twin, we return once again to Fig. 3.4.3.5(*a*) and split the space along the plane *p* into a half-space $\mathcal{B}_1$ on the negative side of the plane *p* (defined by a negative end of normal **n**) and another half-space $\mathcal{B}_2$ on the positive side of *p*. In the parent phase, the whole space is filled with domain state $\mathbf{R}_0$ and we can, therefore, treat the crystal in region $\mathcal{B}_1$ as a domain $\mathbf{D}_1(\mathbf{R}_0, \mathcal{B}_1)$ and the crystal in region $\mathcal{B}_2$ as a domain $\mathbf{D}_2(\mathbf{R}_0, \mathcal{B}_2)$ (we remember that a domain is specified by its domain region, *e.g.* $\mathcal{B}_1$, and by a domain state, *e.g.* $\mathbf{R}_1$, in this region; see Section 3.4.2.1).

Now we cool the crystal down and exert the spontaneous strain $\mathbf{u}^{(1)}$ on domain $\mathbf{D}_1(\mathbf{R}_0, \mathcal{B}_1)$. The resulting domain $\mathbf{D}_1(\mathbf{R}_1, \mathcal{B}_1^-)$ contains domain state $\mathbf{R}_1$ in the domain region $\mathcal{B}_1^-$ with the planar boundary along $(\overline{B_1 C_1})$ (the overbar '−' signifies a rotation of the boundary in the positive sense). Similarly, domain $\mathbf{D}_2(\mathbf{R}_0, \mathcal{B}_2)$ changes after performing spontaneous strain $\mathbf{u}^{(2)}$ into domain $\mathbf{D}_2(\mathbf{R}_2, \mathcal{B}_2^+)$ with domain state $\mathbf{R}_2$ and the planar boundary along $(\overline{B_2 C_2})$. This results in a disruption in the sector $B_1 A B_2$ and in an overlap of $\mathbf{R}_1$ and $\mathbf{R}_2$ in the sector $C_1 A C_2$.

The overlap can be removed and the continuity recovered by rotating the domain $\mathbf{D}_1(\mathbf{R}_1, \mathcal{B}_1^-)$ through angle $\varphi/2$ and the domain $\mathbf{D}_2(\mathbf{R}_2, \mathcal{B}_2^+)$ through $-\varphi/2$ about the domain-pair axis *A* (see Fig. 3.4.3.5*a* and *b*). This rotation changes the domain $\mathbf{D}_1(\mathbf{R}_1, \mathcal{B}_1^-)$ into domain $\mathbf{D}_1(\mathbf{R}_1^+, \mathcal{B}_1)$ and domain $\mathbf{D}_2(\mathbf{R}_2, \mathcal{B}_2^-)$ into domain $\mathbf{D}_1(\mathbf{R}_2^-, \mathcal{B}_2)$, where $\mathbf{R}_1^+$ and $\mathbf{R}_2^-$ are domain states rotated away from the single-domain state orientation through $\varphi/2$ and $-\varphi/2$, respectively. Domains $\mathbf{D}_1(\mathbf{R}_1, \mathcal{B}_1)$ and $\mathbf{D}_1(\mathbf{R}_2, \mathcal{B}_2)$ meet without additional strains or stresses along the plane *p* and form a *simple ferroelastic twin* with a *compatible domain wall* along *p*. This wall is stress-free and fulfils the conditions of mechanical compatibility.

Domain states $\mathbf{R}_1^+$ and $\mathbf{R}_2^-$ with new orientations are called *disoriented (misoriented) domain states* or *suborientational states* (Shuvalov *et al.*, 1985; Dudnik & Shuvalov, 1989) and the angles
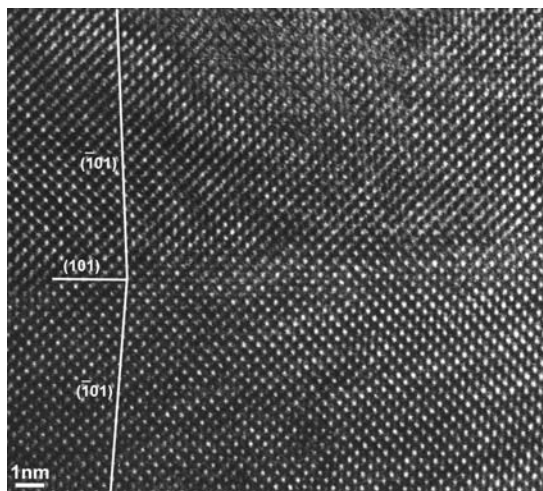
Fig. 3.4.3.6. High-resolution electron microscopy image of a ferroelastic twin in the orthorhombic phase of WO₃. Courtesy of H. Lemmens, EMAT, University of Antwerp.

$\varphi/2$ and $-\varphi/2$ are the *disorientation angles* of $\mathbf{R}_1^+$ and $\mathbf{R}_2^-$, respectively.

We have described the formation of a ferroelastic domain twin by rotating single-domain states into new orientations in which a stress-free compatible contact of two ferroelastic domains is achieved. The advantage of this theoretical construct is that it provides a visual interpretation of disorientations and that it works with ferroelastic single-domain states which can be easily derived and transformed.

There is an alternative approach in which a domain state in one domain is produced from the domain state in the other domain by a shear deformation. The same procedure is used in mechanical twinning [for mechanical twinning, see Section 3.3.8.4 and *e.g.* Cahn (1954); Klassen-Neklyudova (1964); Christian (1975)].

We illustrate this approach again using our example. From Fig. 3.4.3.5(*b*) it follows that domain state $\mathbf{R}_2^-$ in the second domain can be obtained by performing a simple shear on the domain state $\mathbf{R}_1^+$ of the first domain. In this simple shear, a point is displaced in a direction parallel to the equally deformed plane *p* (in mechanical twinning called a *twin plane*) and to a plane perpendicular to the axis of the domain pair (*plane of shear*). The displacement **q** is proportional to the distance *d* of the point from the domain wall. The *amount of shear* is measured either by the absolute value of this displacement at a unit distance, $s = q/d$, or by an angle φ called a *shear angle* (sometimes 2φ is defined as the shear angle). There is no change of volume connected with a simple shear.

The angle φ is also called an *obliquity* of a twin (Cahn, 1954) and is used as a convenient measure of pseudosymmetry of the ferroelastic phase.

The high-resolution electron microscopy image in Fig. 3.4.3.6 reveals the relatively large shear angle (obliquity) φ of a ferroelastic twin in the monoclinic phase of tungsten trioxide (WO₃). The plane (101) corresponds to the plane *p* of a ferroelastic wall in Fig. 3.4.3.5(*b*). The planes ($\overline{1}01$) are crystallographic planes in the lower and upper ferroelastic domains, which correspond in Fig. 3.4.3.5(*b*) to domain $\mathbf{D}_1(\mathbf{R}_1^+, \mathcal{B}_1)$ and domain $\mathbf{D}_2(\mathbf{R}_2^-, \mathcal{B}_2)$, respectively. The planes ($\overline{1}01$) in these domains correspond to the diagonals of the elementary cells of $\mathbf{R}_1^+$ and $\mathbf{R}_2^-$ in Fig. 3.4.3.5(*b*) and are nearly perpendicular to the wall. The angle between these planes equals 2φ, where φ is the shear angle (obliquity) of the ferroelastic twin.

Disorientations of domain states in a ferroelastic twin bring about a deviation of the optical indicatrix from a strictly perpendicular position. Owing to this effect, ferroelastic domains exhibit different colours in polarized light and can be easily visualized. This is illustrated for a domain structure of

(a)

(b)
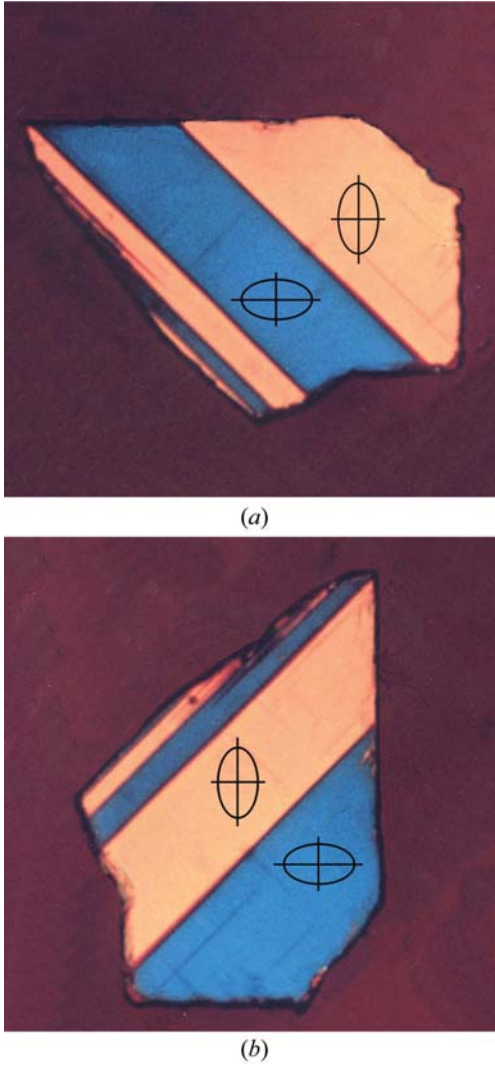
Fig. 3.4.3.7. Ferroelastic twins in a very thin YBa$_2$Cu$_3$O$_{7-\delta}$ crystal observed in a polarized-light microscope. Courtesy of H. Schmid, Université de Geneve.

YBa$_2$Cu$_3$O$_{7-\delta}$ in Fig. 3.4.3.7. The symmetry descent $G = 4_z/m_z m_x m_{xy} \supset m_x m_y m_z = F_1 = F_2$ gives rise to two ferroelastic domain states $\mathbf{R}_1$ and $\mathbf{R}_2$. The twinning group K_{12} of the non-trivial domain pair $(\mathbf{R}_1, \mathbf{R}_2)$ is

$$K_{12}[m_x m_y m_z] = J_{12}^{\star} = m_x m_y m_z \cup 4_z^{\star}\{2_x m_y m_z\} = 4_z^{\star}/m_z m_x m_{xy}^{\star}.$$
(3.4.3.61)

The colour of a domain state observed in a polarized-light microscope depends on the orientation of the index ellipsoid (indicatrix) with respect to a fixed polarizer and analyser. This index ellipsoid transforms in the same way as the tensor of spontaneous strain, *i.e.* it has different orientations in ferroelastic domain states. Therefore, different ferroelastic domain states exhibit different colours: in Fig. 3.4.3.7, the blue and pink areas (with different orientations of the ellipse representing the spontaneous strain in the plane of of figure) correspond to two different ferroelastic domain states. A rotation of the crystal that does not change the orientation of ellipses (*e.g.* a 180° rotation about an axis parallel to the fourfold rotation axis) does not change the colours (ferroelastic domain states). If one neglects disorientations of ferroelastic domain states (see Section 3.4.3.6) – which are too small to be detected by polarized-light microscopy – then none of the operations of the group $F_1 = F_2 = m_x m_y m_z$ change the single-domain ferroelastic domain states $\mathbf{R}_1$, $\mathbf{R}_2$, hence there is no change in the colours of domain regions of the crystal. On the other hand, all operations with a

star symbol (operations lost at the transition) exchange domain states $\mathbf{R}_1$ and $\mathbf{R}_2$, *i.e.* also exchange the two colours in the domain regions. The corresponding permutation is a transposition of two colours and this attribute is represented by a star attached to the symbol of the operation. This exchange of colours is nicely demonstrated in Fig. 3.4.3.7 where a $-90°$ rotation is accompanied by an exchange of the pink and blue colours in the domain regions (Schmid, 1991, 1993).

It can be shown (Shuvalov *et al.*, 1985; Dudnik & Shuvalov, 1989) that for small spontaneous strains the amount of shear s and the angle φ can be calculated from the second invariant Λ_2 of the differential tensor Δu_{ik}:

$$s = 2\sqrt{-\Lambda_2},$$
(3.4.3.62)

$$\varphi = \sqrt{-\Lambda_2},$$
(3.4.3.63)

where

$$\Lambda_2 = \begin{vmatrix} \Delta u_{11} & \Delta u_{12} \\ \Delta u_{21} & \Delta u_{22} \end{vmatrix} + \begin{vmatrix} \Delta u_{22} & \Delta u_{23} \\ \Delta u_{32} & \Delta u_{33} \end{vmatrix} + \begin{vmatrix} \Delta u_{11} & \Delta u_{13} \\ \Delta u_{31} & \Delta u_{33} \end{vmatrix}.$$
(3.4.3.64)

In our example, where there are only two nonzero components of the differential spontaneous strain tensor [see equation (3.4.3.58)], the second invariant $\Lambda_2 = -(\Delta u_{11} \Delta u_{22}) = -(u_{22} - u_{11})^2$ and the angle φ is

$$\varphi = \pm|u_{22} - u_{11}|.$$
(3.4.3.65)

In this case, the angle φ can also be expressed as $\varphi = \pi/2 - 2 \arctan a/b$, where a and b are lattice parameters of the orthorhombic phase (Schmid *et al.*, 1988).

The shear angle φ ranges in ferroelastic crystals from minutes to degrees (see *e.g.* Schmid *et al.*, 1988; Dudnik & Shuvalov, 1989).

Each equally deformed plane gives rise to two compatible domain walls of the same orientation but with opposite sequence of domain states on each side of the plane. We shall use for a *simple domain twin* with a planar wall a symbol $(\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-)$ in which $\mathbf{n}$ denotes the normal to the wall. The bra–ket symbol (| and |) represents the half-space domain regions on the negative and positive sides of $\mathbf{n}$, respectively, for which we have used letters $\mathcal{B}_1$ and $\mathcal{B}_2$, respectively. Then $(\mathbf{R}_1^+|$ and $|\mathbf{R}_2^-)$ represent domains $\mathbf{D}_1(\mathbf{R}_1^+, \mathcal{B}_1)$ and $\mathbf{D}_2(\mathbf{R}_2^-, \mathcal{B}_2)$, respectively. The symbol $(\mathbf{R}_1^+|\mathbf{R}_2^-)$ properly specifies a domain twin with a zero-thickness domain wall.

A domain wall can be considered as a domain twin with domain regions restricted to non-homogeneous parts near the plane p. For a domain wall in domain twin $(\mathbf{R}_1^+|\mathbf{R}_2^-)$ we shall use the symbol $[\mathbf{R}_1^+|\mathbf{R}_2^-]$, which expresses the fact that a domain wall of zero thickness needs the same specification as the domain twin.

If we exchange domain states in the twin $(\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-)$, we get a *reversed twin (wall)* with the symbol $(\mathbf{R}_2^-|\mathbf{n}|\mathbf{R}_1^+)$. These two ferroelastic twins are depicted in the lower right and upper left parts of Fig. 3.4.3.8, where – for ferroelastic–non-ferroelectric twins – we neglect spontaneous polarization of ferroelastic domain states. The reversed twin $\mathbf{R}_2^-|\mathbf{n}'|\mathbf{R}_1^+$ has the opposite shear direction.

Twin and reversed twin can be, but may not be, crystallographically equivalent. Thus *e.g.* ferroelastic–non-ferroelectric twins $(\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-)$ and $(\mathbf{R}_2^-|\mathbf{n}|\mathbf{R}_1^+)$ in Fig. 3.4.3.8 are equivalent, *e.g.* via 2_z, whereas ferroelastic–ferroelectric twins $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_3^-)$ and $(\mathbf{S}_3^-|\mathbf{n}|\mathbf{S}_1^+)$ are not equivalent, since there is no operation in the group K_{12} that would transform $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_3^-)$ into $(\mathbf{S}_3^-|\mathbf{n}|\mathbf{S}_1^+)$.

As we shall show in the next section, the symmetry group $\mathsf{T}_{12}(\mathbf{n})$ of a twin and the symmetry group $\mathsf{T}_{21}(\mathbf{n})$ of a reverse twin are equal,

$$\mathsf{T}_{12}(\mathbf{n}) = \mathsf{T}_{21}(\mathbf{n}).$$
(3.4.3.66)
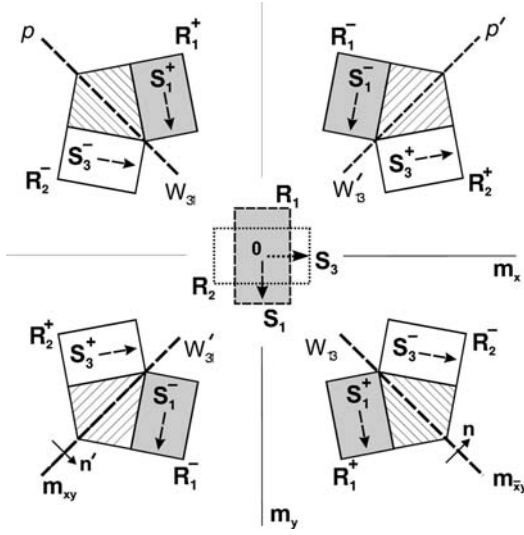
Fig. 3.4.3.8. Exploded view of four ferroelastic twins with disoriented ferroelastic domain states $\mathbf{R}_1^+, \mathbf{R}_2^-$ and $\mathbf{R}_1^-, \mathbf{R}_2^+$ formed from a single-domain pair $(\mathbf{S}_1, \mathbf{S}_2)$ (in the centre).

A sequence of repeating twins and reversed twins

$$\ldots \mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-|\mathbf{n}|\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-|\mathbf{n}|\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-|\mathbf{n}|\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^- \ldots \quad (3.4.3.67)$$

forms a *lamellar ferroelastic domain structure* that is very common in ferroelastic phases (see *e.g.* Figs. 3.4.1.1 and 3.4.1.4).

Similar considerations can be applied to the second equally deformed plane p' that is perpendicular to p. The two twins and corresponding compatible domain walls for the equally deformed plane p' have the symbols $(\mathbf{R}_1^-|\mathbf{n}'|\mathbf{R}_2^+)$ and $(\mathbf{R}_2^-|\mathbf{n}'|\mathbf{R}_1^+)$, and are also depicted in Fig. 3.4.3.8. The corresponding lamellar domain structure is

$$\ldots \mathbf{R}_1^-|\mathbf{n}'|\mathbf{R}_2^+|\mathbf{n}'|\mathbf{R}_1^-|\mathbf{n}'|\mathbf{R}_2^+|\mathbf{n}'|\mathbf{R}_1^-|\mathbf{n}'|\mathbf{R}_2^+|\mathbf{n}'|\mathbf{R}_1^-|\mathbf{n}'|\mathbf{R}_2^+ \ldots .$$
$$(3.4.3.68)$$

Thus from one ferroelastic single-domain pair $(\mathbf{R}_1, \mathbf{R}_2)$ depicted in the centre of Fig. 3.4.3.8 four different ferroelastic domain twins can be formed. It can be shown that these four twins have the same shear angle φ and the same amount of shear s. They differ only in the direction of the shear.

Four disoriented domain states $\mathbf{R}_1^-, \mathbf{R}_1^+$ and $\mathbf{R}_2^-, \mathbf{R}_2^+$ that appear in the four domain twins considered above are related by lost operations (*e.g.* diagonal, vertical and horizontal reflections), *i.e.* they are crystallographically equivalent. This result can readily be obtained if we consider the stabilizer of a disoriented domain state $\mathbf{R}_1^+$, which is $I_{4/mmm}(\mathbf{R}_1^+) = 2_z/m_z$. Then the number n_a^{dis} of disoriented ferroelastic domain states is given by

$$n_a^{\mathrm{dis}} = [G : I_g(\mathbf{R}_1^+)] = |4_z/m_z m_x m_{xy}| : |2_z/m_z| = 16 : 4 = 4.$$
$$(3.4.3.69)$$

All these domain states appear in ferroelastic polydomain structures that contain coexisting lamellar structures (3.4.3.67) and (3.4.3.68).

Disoriented domain states in ferroelastic domain structures can be recognized by diffraction techniques (*e.g.* using an X-ray precession camera). The presence of these four disoriented domain states results in splitting of the diffraction spots of the high-symmetry tetragonal phase into four or two spots in the orthorhombic ferroelastic phase. This splitting is schematically depicted in Fig. 3.4.3.9. For more details see *e.g.* Shmyt'ko *et al.* (1987), Rosová *et al.* (1993), and Rosová (1999).

Finally, we turn to *twin laws of ferroelastic domain twins with compatible domain walls*. In a ferroelastic twin, say $(\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-)$,
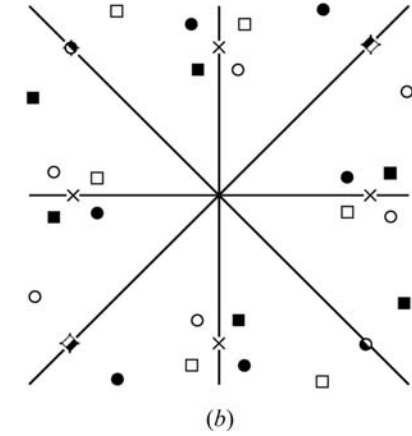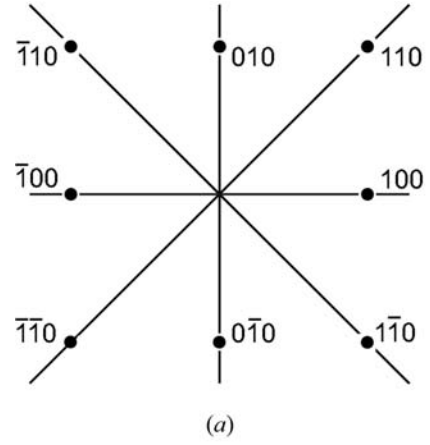
Fig. 3.4.3.9. Splitting of diffraction spots from the four domain twins in Fig. 3.4.3.8. (*a*) Diffraction spots of the tetragonal parent phase of the domain state $\mathbf{R}_1$. (*b*) Diffraction pattern of the domain structure with four domain twins: white circles, $\mathbf{R}_1^+$; black circles, $\mathbf{R}_1^-$; white squares, $\mathbf{R}_2^+$; black squares, $\mathbf{R}_2^-$.

there are just two possible *twinning operations* that interchange two ferroelastic domain states $\mathbf{R}_1^+$ and $\mathbf{R}_2^-$ of the twin: reflection through the plane of the domain wall ($m_{\bar{x}y}^\star$ in our example) and $180°$ rotation with a rotation axis in the intersection of the domain wall and the plane of shear ($2_{xy}^\star$). These are the only transposing operations of the domain pair $(\mathbf{R}_1, \mathbf{R}_2)$ that are preserved by the shear; all other transposing operations of the domain pair $(\mathbf{R}_1, \mathbf{R}_2)$ are lost. (This is a difference from non-ferroelastic twins, where all transposing operations of the pair become twinning operations of a non-ferroelastic twin.)

Consider the twin $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_3^-)$ in Fig. 3.4.3.8. By *non-trivial twinning operations* we understand transposing operations of the domain pair $(\mathbf{S}_1^+, \mathbf{S}_3^-)$, whereas *trivial twinning operations* leave invariant $\mathbf{S}_1^+$ and $\mathbf{S}_3^-$. As we shall see in the next section, the union of trivial and non-trivial twinning operations forms a group $\mathsf{T}_{1+2-}(\mathbf{n})$. This group, called the *symmetry group of the twin* $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_3^-)$, comprises all symmetry operations of this twin and we shall use it for designating the *twin law of the ferroelastic twin*, just as the group $J_{1j}^\star$ of the domain pair $(\mathbf{S}_1, \mathbf{S}_j)$ specifies the twin law of a non-ferroelastic twin. This group $\mathsf{T}_{1+2-}(\mathbf{n})$ is a layer group (see Section 3.4.4.2) that keeps the plane p invariant, but for characterizing the twin law, which specifies the relation of domain states of two domains in the twin, one can treat $\mathsf{T}_{1+2-}(\mathbf{n})$ as an ordinary (dichromatic) point group $T_{1+2-}(\mathbf{n})$. Thus the twin law of the domain twin $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_3^-)$ is designated by the group

$$T_{1+3-}(\mathbf{n}) = 2_{xy}^\star m_{x\bar{y}}^\star m_z = T_{3-1+}(\mathbf{n}), \quad (3.4.3.70)$$

where (3.4.3.70) expresses the fact that a twin and the reversed twin have the same symmetry, see equation (3.4.3.66). We see that

485

this group coincides with the symmetry group J_{1+2-} of the single-domain pair $(\mathbf{S}_1, \mathbf{S}_3)$ (see Fig. 3.4.3.1b).

The twin law of two twins $(\mathbf{S}_1^-|\mathbf{n}'|\mathbf{S}_3^+)$ and $(\mathbf{S}_3^+|\mathbf{n}'|\mathbf{S}_1^-)$ with the same equally deformed plane p' is expressed by the group

$$T_{1-3+}(\mathbf{n}') = m_z = T_{3-1+}(\mathbf{n}'), \qquad (3.4.3.71)$$

which is different from the $T_{1+3-}(\mathbf{n})$ of the twin $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_3^-)$.

Representative domain pairs of all orbits of ferroelastic domain pairs (Litvin & Janovec, 1999) are listed in two tables. Table 3.4.3.6 contains representative domain pairs for which compatible domain walls exist and Table 3.4.3.7 lists ferroelastic domain pairs where compatible coexistence of domain states is not possible. Table 3.4.3.6 contains, beside other data, for each ferroelastic domain pair the orientation of two equally deformed planes and the corresponding symmetries of the corresponding four twins which express two twin laws.

3.4.3.6.4. *Ferroelastic domain pairs with compatible domain walls, synoptic table*

As we have seen, for each ferroelastic domain pair for which condition (3.4.3.54) for the existence of coherent domain walls is fulfilled, there exist two perpendicular equally deformed planes. On each of these planes two ferroelastic twins can be formed; these two twins are in a simple relation (one is a reversed twin of the other), have the same symmetry, and can therefore be represented by one of these twins. Then we can say that from one ferroelastic domain pair two different twins can be formed. Each of these twins represents a different 'twin law' that has arisen from the initial domain pair. All four ferroelastic twins can be described in terms of mechanical twinning with the same value of the shear angle φ.

3.4.3.6.4.1. *Explanation of Table 3.4.3.6*

Table 3.4.3.6 presents representative domain pairs of all classes of ferroelastic domain pairs for which compatible domain walls exist. The first five columns concern the domain pair. In subsequent columns, each row splits into two rows describing the orientation of two associated perpendicular equally deformed planes and the symmetry properties of the four domain twins that can be formed from the given domain pair. We explain the meaning of each column in detail.

The first three columns specify *domain pairs*.

F_1: point-group symmetry (stabilizer in K_{1j}) of the first domain state $\mathbf{S}_1$ in a single-domain orientation.

g_{1j}: switching operations (if available) that specify the domain pair $(\mathbf{S}_1, \mathbf{S}_j = g_{1j}\mathbf{S}_1)$. Subscripts x, y, z specify the orientation of the symmetry operations in the Cartesian coordinate system of K_{1j}. Subscripts x', y' and x'', y'' denote a Cartesian coordinate system rotated about the z axis through 120 and 240°, respectively, from the Cartesian coordinate axes x and y. Diagonal directions are abbreviated: $p = [111]$, $q = [\bar{1}11]$, $r = [1\bar{1}1]$, $s = [11\bar{1}]$. Where possible, reflections and 180° rotations are chosen such that the two perpendicular permissible walls have crystallographic orientations.

K_{1j}: twinning group of the domain pair $(\mathbf{S}_1, \mathbf{S}_j)$. For the pair with $F_1 = m_{x\bar{y}}2_{xy}m_z$ and $K = m\bar{3}m$, where the twinning group does not specify the domain pair unambiguously, we add after K_{1j} in parentheses a switching operation $2_{xz}^\star$ or $m_{xz}^\star$ that defines the domain pair.

Axis: axis of ferroelastic domain pair around which single-domain states must be rotated to establish a contact along a compatible domain wall. This axis is parallel to the intersection of the two compatible domain walls given in the column *Wall*

Table 3.4.3.6. *Ferroelastic domain pairs and twins with compatible walls*

F_1 : symmetry of $\mathbf{S}_1$; g_{1j}: twinning operations; K_{1j}: twinning group; Axis: axis of domain pair; Equation:† direction of the axis; φ:† disorientation angle; $\bar{J}_{1j}$: symmetry of the twin pair; $\underline{t}_{1j}^\star$: twinning operation; $\overline{T}_{1j}$: symmetry of the twin and wall, twin law of the twin; Classification: see Table 3.4.4.3.

F_1	g_{1j}	K_{1j}	Axis	Equation	Wall normals	φ	$\bar{J}_{1j}$	$\underline{t}_{1j}^\star$	$\overline{T}_{1j}$	Classification
1	$2_z^\star$	$2_Z^\star$	$[B\bar{1}0]$	(a)	$[001]$	(1)	$2_z^\star$		1	AR*
					$[1B0]_e$		$\underline{2}_z^\star$	$2_z^\star$	$\underline{2}_z^\star$	SI
1	$m_z^\star$	$m_z^\star$	$[B\bar{1}0]$	(a)	$[001]_e$	(1)	$\underline{m}_z^\star$	$\underline{m}_z^\star$	$\underline{m}_z^\star$	SI
					$[1B0]$		$m_z^\star$		1	AR*
$\bar{1}$	$m_z^\star, 2_z^\star$	$2_z^\star/m_z^\star$	$[B\bar{1}0]$	(a)	$[001]$	(1)	$2_z^\star/\underline{m}_z^\star$	$\underline{m}_z^\star$	$\underline{m}_z^\star$	SR
					$[1B0]$		$\underline{2}_z^\star/m_z^\star$	$\underline{2}_z^\star$	$\underline{2}_z^\star$	SR
2_z	$2_x^\star, 2_y^\star$	$2_x^\star2_y^\star2_z$	$[001]$		$[100]$	(2)	$2_x^\star2_y^\star2_z$	$\underline{2}_y^\star$	$\underline{2}_y^\star$	SR
					$[010]$		$\underline{2}_x^\star\underline{2}_y^\star2_z$	$\underline{2}_x^\star$	$\underline{2}_x^\star$	SR
2_z	$m_x^\star, m_y^\star$	$m_x^\star m_y^\star 2_z$	$[001]$		$[100]$	(2)	$\underline{m}_x^\star m_y^\star 2_z$	$\underline{m}_x^\star$	$\underline{m}_x^\star$	SR
					$[010]$		$m_x^\star\underline{m}_y^\star 2_z$	$\underline{m}_y^\star$	$\underline{m}_y^\star$	SR
2_z	$4_z^\star, 4_z^{3\star}$	$4_z^\star$	$[001]$	(b)	$[1B0]$	(3)	$\underline{2}_z$		1	A$\underline{R}$
					$[B\bar{1}0]$		$\underline{2}_z$		1	A$\underline{R}$
2_z	$\bar{4}_z^\star, \bar{4}_z^{*3}$	$\bar{4}_z^\star$	$[001]$	(b)	$[1B0]$	(3)	$\underline{2}_z$		1	A$\underline{R}$
					$[B\bar{1}0]$		$\underline{2}_z$		1	A$\underline{R}$
2_z	$3_z, 6_z^5$	6_z	$[001]$	(c)	$[1B0]$	(4)	$\underline{2}_z$		1	A$\underline{R}$
					$[B\bar{1}0]$		$\underline{2}_z$		1	A$\underline{R}$
	$3_z^2, 6_z$	6_z	$[001]$	(c)	$[1B0]$	(4)	$\underline{2}_z$		1	A$\underline{R}$
					$[B\bar{1}0]$		$\underline{2}_z$		1	A$\underline{R}$
2_z	$\bar{3}_z^5, \bar{6}_z$	$6_z/m_z$	$[001]$	(c)	$[1B0]$	(4)	$\underline{2}_z$		1	A$\underline{R}$
					$[B\bar{1}0]$		$\underline{2}_z$		1	A$\underline{R}$
	$\bar{3}_z, \bar{6}_z^5$	$6_z/m_z$	$[001]$	(c)	$[1B0]$	(4)	$\underline{2}_z$		1	A$\underline{R}$
					$[B\bar{1}0]$		$\underline{2}_z$		1	A$\underline{R}$
2_x	$2_{xy}^\star, 4_z$	$4_z2_x2_{xy}$	$[\bar{C}C2]$	(d)	$[110]$	(5)	$2_{xy}^\star$		1	AR*
					$[11C]_e$		$\underline{2}_{xy}^\star$	$\underline{2}_{xy}^\star$	$\underline{2}_{xy}^\star$	SI
2_x	$m_{xy}^\star, \bar{4}_z$	$\bar{4}_z2_xm_{xy}$	$[\bar{C}C2]$	(d)	$[110]_e$	(5)	$\underline{m}_{xy}^\star$	$\underline{m}_{xy}^\star$	$\underline{m}_{xy}^\star$	SI
					$[1\bar{1}C]$		$m_{xy}^\star$		1	AR*
2_x	$2_{x'}^\star, 3_z^2$	3_z2_x	$[\sqrt{3}C, C, \bar{4}]$	(e)	$[\bar{1}\sqrt{3}0]$	(6)	$2_{x'}^\star$		1	AR*
					$[\sqrt{3}1C]_e$		$\underline{2}_{x'}^\star$	$\underline{2}_{x'}^\star$	$\underline{2}_{x'}^\star$	SI

Table 3.4.3.6 (*cont.*)

F_1	g_{1j}	K_{1j}	Axis	Equation	Wall normals	φ	$\overline{J}_{1j}$	$\underline{t}_{1j}^\star$	$\overline{T}_{1j}$	Classification
2_x	$m_x^\star, \bar{3}_z^5$	$\bar{3}_z m_x$	$[\sqrt{3}C, C, \bar{4}]$	(e)	$[\bar{1}\sqrt{3}0]_e$ $[\sqrt{3}1C]$	(6)	$\underline{m}_{x'}^\star$ $\underline{m}_{x'}^\star$	$\underline{m}_{x'}^\star$	$\underline{m}_{x'}^\star$ 1	SI AR*
2_x	$2_{y'}^\star, 6_z$	$6_z2_xm_y$	$[\bar{C}, \sqrt{3}C, \bar{4}]$	(f)	$[\sqrt{3}10]$ $[\bar{1}\sqrt{3}C]_e$	(7)	$2_{y'}^\star$ $\underline{2}_{y'}^\star$	$\underline{2}_{y'}^\star$	1 $\underline{2}_{y'}^\star$	AR* SI
2_x	$m_{y'}^\star, \bar{6}_z$	$\bar{6}_z2_xm_y$	$[\bar{C}, \sqrt{3}C, \bar{4}]$	(f)	$[\sqrt{3}10]_e$ $[1\sqrt{3}C]$	(7)	$\underline{m}_{y'}^\star$ $\underline{m}_{y'}^\star$	$\underline{m}_{y'}^\star$	$\underline{m}_{y'}^\star$ 1	SI AR*
2_{xy}	$m_x^\star, \bar{4}_z^3$	$\bar{4}_zm_x2_{xy}$	$[0C\bar{1}]$	(g)	$[100]_e$ $[01C]$	(8)	$\underline{m}_x^\star$ $\underline{m}_x^\star$	$\underline{m}_x^\star$	$\underline{m}_x^\star$ 1	SI AR*
m_z	$m_x^\star, 2_y^\star$	$m_x^\star2_y^\star m_z$	$[001]$		$[100]_e$ $[010]$	(2)	$\underline{m}_x^\star\underline{2}_y^\star m_z$ $m_x^\star2_y^\star m_z$	$\underline{m}_x^\star$	$\underline{m}_x^\star\underline{2}_y^\star m_z$ m_z	SI AR*
m_z	$4_z, \bar{4}_z^3$	$4_z/m_z$	$[001]$	(b)	$[1B0]_{e0}$ $[B\bar{1}0]_{0e}$	(3)	m_z m_z		m_z m_z	AI AI
	$4_z^3, \bar{4}_z$	$4_z/m_z$	$[001]$	(b)	$[1B0]_{e0}$ $[B\bar{1}0]_{0e}$	(3)	m_z m_z		m_z m_z	AI AI
m_z	$3_z, \bar{6}_z^5$	$\bar{6}_z$	$[001]$	(c)	$[1B0]_{e0}$ $[B\bar{1}0]_{0e}$	(4)	m_z m_z		m_z m_z	AI AI
	$3_z^2, \bar{6}_z$	$\bar{6}_z$	$[001]$	(c)	$[1B0]_{e0}$ $[B\bar{1}0]_{0e}$	(4)	m_z m_z		m_z m_z	AI AI
m_z	$\bar{3}_z, 6_z^5$	$6_z/m_z$	$[001]$	(c)	$[1B0]_{e0}$ $[B\bar{1}0]_{0e}$	(4)	m_z m_z		m_z m_z	AI AI
	$\bar{3}_z^5, 6_z$	$6_z/m_z$	$[001]$	(c)	$[1B0]_{e0}$ $[B\bar{1}0]_{0e}$	(4)	m_z m_z		m_z m_z	AI AI
m_x	$m_{xy}^\star, 4_z$	$4_zm_xm_{xy}$	$[\bar{C}C2]$	(d)	$[110]_e$ $[1\bar{1}C]$	(5)	$\underline{m}_{xy}^\star$ $m_{xy}^\star$	$\underline{m}_{xy}^\star$	$\underline{m}_{xy}^\star$ 1	SI AR*
m_x	$2_{xy}^\star, \bar{4}_z$	$\bar{4}_zm_x2_{xy}$	$[\bar{C}C2]$	(d)	$[110]$ $[1\bar{1}C]_e$	(5)	$2_{xy}^\star$ $\underline{2}_{xy}^\star$	$\underline{2}_{xy}^\star$	1 $\underline{2}_{xy}^\star$	AR* SI
m_x	$m_{x'}^\star, 3_z^2$	3_zm_x	$[\sqrt{3}C, C, \bar{4}]$	(e)	$[\bar{1}\sqrt{3}0]_e$ $[\sqrt{3}1C]$	(6)	$\underline{m}_{x'}^\star$ $m_{x'}^\star$	$\underline{m}_{x'}^\star$	$\underline{m}_{x'}^\star$ 1	SI AR*
m_x	$2_{x'}^\star, \bar{3}_z^5$	$\bar{3}_zm_x$	$[\sqrt{3}C, C, \bar{4}]$	(e)	$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}1C]_e$	(6)	$2_{x'}^\star$ $\underline{2}_{x'}^\star$	$\underline{2}_{x'}^\star$	1 $\underline{2}_{x'}^\star$	AR* SI
m_x	$m_{y'}^\star, 6_z$	$6_zm_xm_y$	$[\bar{C}, \sqrt{3}C, \bar{4}]$	(f)	$[\sqrt{3}10]_e$ $[1\sqrt{3}C]$	(7)	$\underline{m}_{y'}^\star$ $m_{y'}^\star$	$\underline{m}_{y'}^\star$	$\underline{m}_{y'}^\star$ 1	SI AR*
m_x	$2_{y'}^\star, \bar{6}_z$	$\bar{6}_zm_x2_y$	$[\bar{C}, \sqrt{3}C, \bar{4}]$	(f)	$[\sqrt{3}10]$ $[\bar{1}\sqrt{3}C]_e$	(7)	$2_{y'}^\star$ $\underline{2}_{y'}^\star$	$\underline{2}_{y'}^\star$	1 $\underline{2}_{y'}^\star$	AR* SI
m_{xy}	$2_x^\star, \bar{4}_z^3$	$\bar{4}_z2_xm_{xy}$	$[0C\bar{1}]$	(g)	$[100]$ $[01C]_e$	(8)	$2_x^\star$ $\underline{2}_{xy}^\star$	$\underline{2}_x^\star$	1 $\underline{2}_x^\star$	AR* SI
$2_z/m_z$	$m_x^\star, m_y^\star$	$m_x^\star m_y^\star m_z$	$[001]$		$[100]$ $[010]$	(2)	$\underline{m}_x^\star m_y^\star m_z$ $m_x^\star\underline{m}_y^\star m_z$	$\underline{m}_x^\star$ $\underline{m}_y^\star$	$\underline{m}_x^\star\underline{2}_y^\star m_z$ $\underline{2}_x^\star\underline{m}_y^\star m_z$	SR SR
$2_z/m_z$	$4_z^\star, 4_z^{3\star}$	$4_z^\star/m_z$	$[001]$	(b)	$[1B0]$ $[B\bar{1}0]$	(3)	$\underline{2}_z/m_z$ $\underline{2}_z/m_z$		m_z m_z	A$\underline{R}$ A$\underline{R}$
$2_z/m_z$	$3_z, 6_z^5$	$6_z/m_z$	$[001]$	(c)	$[1B0]$ $[B\bar{1}0]$	(4)	$\underline{2}_z/m_z$ $\underline{2}_z/m_z$		m_z m_z	A$\underline{R}$ A$\underline{R}$
	$3_z^2, 6_z$	$6_z/m_z$	$[001]$	(c)	$[1B0]$ $[B\bar{1}0]$	(4)	$\underline{2}_z/m_z$ $\underline{2}_z/m_z$		m_z m_z	A$\underline{R}$ A$\underline{R}$
$2_x/m_x$	$m_{xy}^\star, 4_z$	$4_z/m_zm_xm_{xy}$	$[\bar{C}C2]$	(d)	$[110]$ $[1\bar{1}C]$	(5)	$2_{xy}/\underline{m}_{xy}^\star$ $\underline{2}_{xy}/m_{xy}^\star$	$\underline{m}_{xy}^\star$ $\underline{2}_{xy}^\star$	$\underline{m}_{xy}^\star$ $\underline{2}_{xy}^\star$	SR SR
$2_x/m_x$	$m_{x'}^\star, 3_z^2$	$\bar{3}_zm_x$	$[\sqrt{3}CC\bar{4}]$	(e)	$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}1C]$	(6)	$2_{x'}/\underline{m}_{x'}^\star$ $\underline{2}_{x'}/m_{x'}^\star$	$\underline{m}_{x'}^\star$ $\underline{2}_{x'}^\star$	$\underline{m}_{x'}^\star$ $\underline{2}_{x'}^\star$	SR SR
$2_x/m_x$	$m_{y'}^\star, 6_z$	$6_z/m_zm_xm_y$	$[\bar{C}, \sqrt{3}C, \bar{4}]$	(f)	$[\sqrt{3}10]$ $[1\sqrt{3}C]$	(7)	$2_{y'}/\underline{m}_{y'}^\star$ $\underline{2}_{y'}/m_{y'}^\star$	$\underline{m}_{y'}^\star$ $\underline{2}_{y'}^\star$	$\underline{m}_{y'}^\star$ $\underline{2}_{y'}^\star$	SR SR
$2_x2_y2_z$	$2_{x\bar{y}}^\star, 2_{xy}^\star$	$4_z^\star2_x2_{xy}^\star$	$[001]$		$[110]$ $[1\bar{1}0]$	(10)	$2_{xy}2_{x\bar{y}}^\star2_z$ $\underline{2}_{xy}2_{x\bar{y}}^\star2_z$	$\underline{2}_{x\bar{y}}^\star$ $\underline{2}_{xy}^\star$	$\underline{2}_{x\bar{y}}^\star$ $\underline{2}_{xy}^\star$	SR SR
$2_x2_y2_z$	$m_{x\bar{y}}^\star, m_{xy}^\star$	$\bar{4}_z^\star2_xm_{xy}^\star$	$[001]$		$[110]$ $[1\bar{1}0]$	(10)	$\underline{m}_{xy}m_{x\bar{y}}^\star\underline{2}_z$ $m_{xy}^\star\underline{m}_{x\bar{y}}\underline{2}_z$	$\underline{m}_{xy}^\star$ $\underline{m}_{x\bar{y}}^\star$	$\underline{m}_{xy}^\star$ $\underline{m}_{x\bar{y}}^\star$	SR SR
$2_x2_y2_z$	$2_{x'}^\star, 2_{y'}^\star$	$6_z2_x2_y$	$[001]$		$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}10]$	(9)	$2_{x'}^\star2_{y'}^\star2_z$ $\underline{2}_{x'}^\star2_{y'}^\star2_z$	$\underline{2}_{y'}^\star$ $\underline{2}_{x'}^\star$	$\underline{2}_{y'}^\star$ $\underline{2}_{x'}^\star$	SR SR
$2_x2_y2_z$	$m_{x'}^\star, m_{y'}^\star$	$6_z/m_zm_xm_y$	$[001]$		$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}10]$	(9)	$\underline{m}_{x'}^\star m_{y'}^\star\underline{2}_z$ $m_{x'}^\star\underline{m}_{y'}^\star\underline{2}_z$	$\underline{m}_{x'}^\star$ $\underline{m}_{y'}^\star$	$\underline{m}_{x'}^\star$ $\underline{m}_{y'}^\star$	SR SR
$2_{x\bar{y}}2_{xy}2_z$	$m_x^\star, m_y^\star$	$\bar{4}_z^\star m_x^\star2_{xy}$	$[001]$		$[100]$ $[010]$	(12)	$\underline{m}_x^\star m_y^\star\underline{2}_z$ $m_x^\star\underline{m}_y^\star\underline{2}_z$	$\underline{m}_x^\star$ $\underline{m}_y^\star$	$\underline{m}_x^\star$ $\underline{m}_y^\star$	SR SR

Table 3.4.3.6 (*cont.*)

F_1	g_{1j}	K_{1j}	Axis	Equation	Wall normals	φ	$\overline{J}_{1j}$	$\underline{t}_{1j}^\star$	$\overline{T}_{1j}$	Classification
$2_{x\bar{y}}2_{xy}2_z$	$2_{xz}^\star, 4_y$	$4_z3_p2_{xy}$	$[B2\bar{B}]$	(h)	$[101]$ $[\bar{1}B1]$	(11)	$2_{xz}^\star$ $2_{xz}^\star$	$2_{xz}^\star$	1 $2_{xz}^\star$	AR* SI
$2_{x\bar{y}}2_{xy}2_z$	$m_{xz}^\star, \bar{4}_y$	$m_z\bar{3}_pm_{xy}$	$[B2\bar{B}]$	(h)	$[101]$ $[\bar{1}B1]$	(11)	$\underline{m}_{xz}^\star$ $m_{xz}^\star$	$\underline{m}_{xz}^\star$	$\underline{m}_{xz}^\star$ 1	SI AR*
$m_xm_y2_z$	$m_{x\bar{y}}^\star, m_{xy}^\star$	$4_z^\star m_xm_{xy}^\star$	$[001]$		$\left[\begin{array}{c}[110] \\ [1\bar{1}0]\end{array}\right.$	(10)	$m_{x\bar{y}}^\star\underline{m}_{xy}^\star\underline{2}_z$ $\underline{m}_{x\bar{y}}^\star m_{xy}^\star\underline{2}_z$	$\underline{m}_{xy}^\star$ $\underline{m}_{x\bar{y}}^\star$	$\underline{m}_{xy}^\star$ $\underline{m}_{x\bar{y}}^\star$	SR SR
$m_xm_y2_z$	$2_{x\bar{y}}^\star, 2_{xy}$	$\bar{4}_z^\star m_x2_{xy}$	$[001]$		$\left[\begin{array}{c}[110] \\ [1\bar{1}0]\end{array}\right.$	(10)	$2_{x\bar{y}}^\star\underline{2}_{xy}^\star\underline{2}_z$ $\underline{2}_{x\bar{y}}^\star2_{x\bar{y}}^\star\underline{2}_z$	$2_{x\bar{y}}^\star$ $2_{xy}^\star$	$2_{x\bar{y}}^\star$ $2_{xy}^\star$	SR SR
$m_xm_y2_z$	$m_{x'}^\star, m_{y'}^\star$	$6_z m_xm_y$	$[001]$		$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}10]$	(9)	$\underline{m}_{x'}^\star m_{y'}^\star\underline{2}_z$ $m_{x'}^\star\underline{m}_{y'}^\star\underline{2}_z$	$\underline{m}_{x'}^\star$ $\underline{m}_{y'}^\star$	$\underline{m}_{x'}^\star$ $\underline{m}_{y'}^\star$	SR SR
$m_xm_y2_z$	$2_{x'}^\star, 2_{y'}^\star$	$6_z/m_zm_xm_y$	$[001]$		$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}10]$	(9)	$2_{x'}^\star\underline{2}_{y'}^\star\underline{2}_z$ $\underline{2}_{x'}^\star2_{y'}^\star\underline{2}_z$	$2_{y'}^\star$ $2_{x'}^\star$	$2_{y'}^\star$ $2_{x'}^\star$	SR SR
$m_x2_ym_z$	$m_{x'}^\star, 2_{y'}^\star$	$\bar{6}_z m_x2_y$	$[001]$		$[\bar{1}\sqrt{3}0]_e$ $[\sqrt{3}10]$	(9)	$\underline{m}_{x'}^\star\underline{2}_{y'}^\star m_z$ $m_{x'}^\star\underline{2}_{y'}^\star m_z$	$\underline{m}_{x'}^\star$	$\underline{m}_{x'}^\star\underline{2}_{y'}^\star m_z$ m_z	SI AR*
$2_xm_ym_z$	$m_{x\bar{y}}^\star, 2_{xy}$	$4_z/m_zm_xm_{xy}$	$[001]$		$[110]$ $[1\bar{1}0]_e$	(10)	$2_{xy}m_{x\bar{y}}^\star m_z$ $\underline{2}_{xy}^\star\underline{m}_{x\bar{y}}^\star m_z$	$\underline{m}_{x\bar{y}}^\star$	m_z $\underline{2}_{xy}^\star\underline{m}_{x\bar{y}}^\star m_z$	AR* SI
$2_xm_ym_z$	$m_{y'}^\star, 2_{x'}^\star$	$\bar{6}_z2_xm_y$	$[001]$		$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}10]_e$	(9)	$2_{x'}^\star m_{y'}^\star m_z$ $\underline{2}_{x'}^\star\underline{m}_{y'}^\star m_z$	$m_{y'}$	m_z $\underline{2}_{x'}^\star\underline{m}_{y'}^\star m_z$	AR* SI
$2_xm_ym_z$	$m_{x'}^\star, 2_{y'}^\star$	$6_z/m_zm_xm_y$	$[001]$		$[\bar{1}\sqrt{3}0]_e$ $[\sqrt{3}10]$	(9)	$\underline{m}_{x'}^\star\underline{2}_{y'}^\star m_z$ $m_{x'}^\star\underline{2}_{y'}^\star m_z$	$\underline{m}_{x'}^\star$	$\underline{m}_{x'}^\star\underline{2}_{y'}^\star m_z$ m_z	SI AR*
$m_{x\bar{y}}m_{xy}2_z$	$2_x^\star, 2_y^\star$	$\bar{4}_z^\star2_x^\star m_{xy}$	$[001]$		$\left[\begin{array}{c}[100] \\ [010]\end{array}\right.$	(12)	$2_x^\star2_y^\star\underline{2}_z$ $\underline{2}_x^\star2_y^\star\underline{2}_z$	$2_y^\star$ $2_x^\star$	$2_y^\star$ $2_x^\star$	SR SR
$m_{x\bar{y}}m_{xy}2_z$	$m_{xz}^\star, \bar{4}_y$	$\bar{4}_z3_pm_{xy}$	$[B2\bar{B}]$	(h)	$[101]_e$ $[\bar{1}B1]$	(11)	$\underline{m}_{xz}^\star$ $m_{xz}^\star$	$\underline{m}_{xz}^\star$	$\underline{m}_{xz}^\star$ 1	SI AR*
$m_{x\bar{y}}m_{xy}2_z$	$2_{xz}^\star, 4_y$	$m_z\bar{3}_pm_{xy}$	$[B2\bar{B}]$	(h)	$[101]$ $[\bar{1}B1]_e$	(11)	$2_{xz}^\star$ $2_{xz}^\star$	$2_{xz}^\star$	1 $2_{xz}^\star$	AR* SI
$m_{x\bar{y}}2_{xy}m_z$	$m_{xz}^\star, 4_y$	$m_z\bar{3}_pm_{xy}(m_{xz}^\star)$	$[B2\bar{B}]$	(h)	$[101]_e$ $[\bar{1}B1]$	(11)	$\underline{m}_{xz}^\star$ $m_{xz}^\star$	$\underline{m}_{xz}^\star$	$\underline{m}_{xz}^\star$ 1	SI AR*
$m_{x\bar{y}}2_{xy}m_z$	$2_{xz}^\star, \bar{4}_y$	$m_z\bar{3}_pm_{xy}(2_{xz}^\star)$	$[B2\bar{B}]$	(h)	$[101]$ $[\bar{1}B1]_e$	(11)	$2_{xz}^\star$ $2_{xz}^\star$	$2_{xz}^\star$	1 $2_{xz}^\star$	AR* SI
$m_xm_ym_z$	$m_{xy}^\star, m_{x\bar{y}}^\star$	$4_z^\star/m_zm_xm_{xy}^\star$	$[001]$		$\left[\begin{array}{c}[110] \\ [1\bar{1}0]\end{array}\right.$	(10)	$m_{x\bar{y}}^\star\underline{m}_{xy}^\star m_z$ $\underline{m}_{x\bar{y}}^\star m_{xy}^\star m_z$	$\underline{m}_{xy}^\star$ $\underline{m}_{x\bar{y}}^\star$	$\underline{2}_{x\bar{y}}^\star\underline{m}_{xy}^\star m_z$ $\underline{m}_{x\bar{y}}^\star\underline{2}_{xy}^\star m_z$	SR SR
$m_xm_ym_z$	$m_{x'}^\star, m_{y'}^\star$	$6_z/m_zm_xm_y$	$[001]$		$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}10]$	(9)	$\underline{m}_{x'}^\star m_{y'}^\star m_z$ $m_{x'}^\star\underline{m}_{y'}^\star m_z$	$\underline{m}_{x'}^\star$ $\underline{m}_{y'}^\star$	$\underline{m}_{x'}^\star\underline{2}_{y'}^\star m_z$ $\underline{2}_{x'}^\star\underline{m}_{y'}^\star m_z$	SR SR
$m_{xy}m_{\bar{x}y}m_z$	$m_{xz}^\star, 4_y$	$m_z\bar{3}_pm_{xy}$	$[B2\bar{B}]$	(h)	$[101]$ $[\bar{1}B1]$	(11)	$2_{xz}^\star/\underline{m}_{xz}^\star$ $\underline{2}_{xz}^\star/m_{xz}^\star$	$\underline{m}_{xz}^\star$ $2_{xz}^\star$	$\underline{m}_{xz}^\star$ $2_{xz}^\star$	SR SR
4_z	$2_{xz}^\star, 4_y$	$4_z3_p2_{xy}$	$[010]$		$[101]$ $[\bar{1}01]_e$	(13)	$2_{xz}^\star$ $2_{xz}^\star$	$2_{xz}^\star$	1 $2_{xz}^\star$	AR* SI
4_z	$m_{xz}^\star, \bar{4}_y$	$m_z\bar{3}_pm_{xy}$	$[010]$		$[\bar{1}01]_e$ $[101]$	(13)	$\underline{m}_{xz}^\star$ $m_{xz}^\star$	$\underline{m}_{xz}^\star$	$\underline{m}_{xz}^\star$ 1	SI AR*
$\bar{4}_z$	$m_{xz}^\star, \bar{4}_y$	$\bar{4}_z3_pm_{xy}$	$[010]$		$[\bar{1}01]$ $[101]$	(13)	$\underline{m}_{xz}^\star$ $m_{xz}^\star$	$\underline{m}_{xz}^\star$	$\underline{m}_{xz}^\star$ 1	SI AR*
$\bar{4}_z$	$2_{xz}^\star, 4_y$	$m_z\bar{3}_pm_{xy}$	$[010]$		$[101]$ $[\bar{1}01]_e$	(13)	$2_{xz}^\star$ $2_{xz}^\star$	$2_{xz}^\star$	1 $2_{xz}^\star$	AR* SI
$4_z/m_z$	$m_{xz}^\star, 4_y$	$m_z\bar{3}_pm_{xy}$	$[010]$		$[101]$ $[\bar{1}01]$	(13)	$2_{xz}^\star/\underline{m}_{xz}^\star$ $\underline{2}_{xz}^\star/m_{xz}^\star$	$\underline{m}_{xz}^\star$ $2_{xz}^\star$	$\underline{m}_{xz}^\star$ $2_{xz}^\star$	SR SR
$4_z2_x2_{xy}$	$2_{xz}^\star, 2_{x\bar{z}}$	$4_z3_p2_{xy}$	$[010]$		$\left[\begin{array}{c}[101] \\ [\bar{1}01]\end{array}\right.$	(13)	$2_{xz}^\star\underline{2}_{x\bar{z}}^\star2_y$ $\underline{2}_{xz}^\star2_{x\bar{z}}^\star2_y$	$2_{x\bar{z}}^\star$ $2_{xz}^\star$	$2_{x\bar{z}}^\star$ $2_{xz}^\star$	SR SR
$4_z2_x2_{xy}$	$m_{xz}^\star, m_{x\bar{z}}^\star$	$m_z\bar{3}_pm_{xy}$	$[010]$		$\left[\begin{array}{c}[101] \\ [\bar{1}01]\end{array}\right.$	(13)	$\underline{m}_{xz}^\star m_{x\bar{z}}^\star2_y$ $m_{xz}^\star\underline{m}_{x\bar{z}}^\star2_y$	$\underline{m}_{xz}^\star$ $\underline{m}_{x\bar{z}}^\star$	$\underline{m}_{xz}^\star$ $\underline{m}_{x\bar{z}}^\star$	SR SR
$4_zm_xm_{xy}$	$m_{x\bar{z}}^\star, 2_{xz}^\star$	$m_z\bar{3}_pm_{xy}$	$[010]$		$[\bar{1}01]$ $[\bar{1}01]_e$	(13)	$2_{xz}^\star m_{x\bar{z}}^\star m_y$ $\underline{2}_{xz}^\star\underline{m}_{x\bar{z}}^\star m_y$	$\underline{2}_{xz}^\star$	m_y $\underline{2}_{xz}^\star\underline{m}_{x\bar{z}}^\star m_y$	AR* SI
$\bar{4}_z2_xm_{xy}$	$m_{xz}^\star, m_{x\bar{z}}$	$\bar{4}_z3_pm_{xy}$	$[010]$		$\left[\begin{array}{c}[101] \\ [\bar{1}01]\end{array}\right.$	(13)	$\underline{m}_{xz}^\star m_{x\bar{z}}^\star2_y$ $m_{xz}^\star\underline{m}_{x\bar{z}}^\star2_y$	$\underline{m}_{xz}^\star$ $\underline{m}_{x\bar{z}}^\star$	$\underline{m}_{xz}^\star$ $\underline{m}_{x\bar{z}}^\star$	SR SR
$\bar{4}_zm_x2_{xy}$	$m_{x\bar{z}}^\star, 2_{xz}^\star$	$m_z\bar{3}_pm_{xy}$	$[010]$		$[101]$ $[\bar{1}01]$	(13)	$2_{xz}^\star m_{x\bar{z}}^\star m_y$ $\underline{2}_{xz}^\star\underline{m}_{x\bar{z}}^\star m_y$	$\underline{m}_{x\bar{z}}^\star$	m_y $\underline{2}_{xz}^\star\underline{m}_{x\bar{z}}^\star m_y$	AR* SR
$\bar{4}_z2_xm_{xy}$	$2_{xz}^\star, 2_{x\bar{z}}$	$m_z\bar{3}_pm_{xy}$	$[010]$		$[101]$ $[\bar{1}01]$	(13)	$2_{xz}^\star2_{x\bar{z}}^\star2_y$ $\underline{2}_{xz}^\star\underline{2}_{x\bar{z}}^\star2_y$	$2_{x\bar{z}}^\star$ $2_{x\bar{z}}^\star$	$2_{x\bar{z}}^\star$ $\underline{2}_{xz}^\star\underline{2}_{x\bar{z}}^\star2_y$	SR SI

Table 3.4.3.6 (*cont.*)

F_1	g_{1j}	K_{1j}	Axis	Equation	Wall normals	φ	$\overline{\mathsf{J}}_{1j}$	$t^\star_{1j}$	$\overline{\mathsf{T}}_{1j}$	Classification
$4_z/m_z m_x m_{xy}$	$m^\star_{xz},\,m^\star_{\bar{x}z}$	$m_z\bar{3}_p m_{xy}$	[010]		$\left[\begin{array}{l}[101]\\ [\bar{1}01]\end{array}\right.$	(13)	$\begin{array}{l}m^\star_{xz}m^\star_{\bar{x}z}m_y\\ m^\star_{xz}\underline{m}^\star_{\bar{x}z}m_y\end{array}$	$\begin{array}{l}m^\star_{xz}\\ \underline{m}^\star_{x\bar{z}}\end{array}$	$\begin{array}{l}m^\star_{xz}2^\star_{\bar{x}z}m_y\\ 2^\star_{xz}\underline{m}^\star_{xz}m_y\end{array}$	SR SR
3_p	$2^\star_x,\,3_r$	2_z3_p	$[01\bar{1}]$		$\begin{array}{l}[100]\\ [011]_e\end{array}$	(14)	$\begin{array}{l}2^\star_x\\ \underline{2}^\star_x\end{array}$	$\underline{2}^\star_x$	$\begin{array}{l}1\\ 2^\star_x\end{array}$	AR* SI
3_p	$m^\star_x,\,\bar{3}_r$	$m_z\bar{3}_p$	$[01\bar{1}]$		$\begin{array}{l}[100]_e\\ [011]\end{array}$	(14)	$\begin{array}{l}\underline{m}^\star_x\\ m^\star_x\end{array}$	$\underline{m}^\star_x$	$\begin{array}{l}m^\star_x\\ 1\end{array}$	SI AR*
3_p	$2^\star_{xy},\,4_y$	$4_z3_p2_{xy}$	$[1\bar{1}0]$		$\begin{array}{l}[001]_e\\ [110]\end{array}$	(14)	$\begin{array}{l}\underline{2}^\star_{xy}\\ 2^\star_{xy}\end{array}$	$\underline{2}^\star_{xy}$	$\begin{array}{l}2^\star_{xy}\\ 1\end{array}$	SI AR*
3_p	$m^\star_{xy},\,\bar{4}_y$	$\bar{4}_z3_p m_{xy}$	$[1\bar{1}0]$		$\begin{array}{l}[001]\\ [110]_e\end{array}$	(14)	$\begin{array}{l}m^\star_{xy}\\ \underline{m}^\star_{xy}\end{array}$	$\underline{m}^\star_{xy}$	$\begin{array}{l}1\\ m^\star_{xy}\end{array}$	AR* SI
$\bar{3}_p$	$m^\star_x,\,3_r$	$m_z\bar{3}_p$	$[01\bar{1}]$		$\begin{array}{l}[100]\\ [011]\end{array}$	(14)	$\begin{array}{l}2^\star_x/\underline{m}^\star_x\\ \underline{2}^\star_x/m^\star_x\end{array}$	$\begin{array}{l}\underline{m}^\star_x\\ \underline{2}^\star_x\end{array}$	$\begin{array}{l}m^\star_x\\ 2^\star_x\end{array}$	SR SR
$\bar{3}_p$	$m^\star_{xy},\,4_y$	$m_z\bar{3}_p m_{xy}$	$[1\bar{1}0]$		$\begin{array}{l}[001]\\ [110]\end{array}$	(14)	$\begin{array}{l}2^\star_{xy}/m^\star_{xy}\\ \underline{2}^\star_{xy}/\underline{m}^\star_{xy}\end{array}$	$\begin{array}{l}2^\star_{xy}\\ \underline{m}^\star_{xy}\end{array}$	$\begin{array}{l}2^\star_{xy}\\ \underline{m}^\star_{xy}\end{array}$	SR SR
$3_p2_{x\bar{y}}$	$2^\star_x,\,2^\star_{yz}$	$4_z3_p2_{xy}$	$[01\bar{1}]$		$\begin{array}{l}[100]\\ [011]\end{array}$	(14)	$\begin{array}{l}2^\star_x2^\star_{yz}\underline{2}_{y\bar{z}}\\ \underline{2}^\star_x2^\star_{yz}\underline{2}_{y\bar{z}}\end{array}$	$\begin{array}{l}\underline{2}^\star_{yz}\\ \underline{2}^\star_x\end{array}$	$\begin{array}{l}2^\star_{yz}\\ 2^\star_x\end{array}$	SR SR
$3_p2_{x\bar{y}}$	$m^\star_x,\,m^\star_{yz}$	$m_z\bar{3}_p m_{xy}$	$[01\bar{1}]$		$\begin{array}{l}[100]\\ [011]\end{array}$	(14)	$\begin{array}{l}\underline{m}^\star_x m^\star_{yz}\underline{2}_{y\bar{z}}\\ m^\star_x\underline{m}^\star_{yz}\underline{2}_{y\bar{z}}\end{array}$	$\begin{array}{l}\underline{m}^\star_x\\ \underline{m}^\star_{yz}\end{array}$	$\begin{array}{l}\underline{m}^\star_x\\ \underline{m}^\star_{yz}\end{array}$	SR SR
$3_p m_{x\bar{y}}$	$2^\star_x,\,m^\star_{yz}$	$\bar{4}_z3_p m_{xy}$	$[01\bar{1}]$		$\begin{array}{l}[100]\\ [011]_e\end{array}$	(14)	$\begin{array}{l}m^\star_{yz}m_{y\bar{z}}2^\star_x\\ \underline{m}^\star_{yz}m_{y\bar{z}}\underline{2}^\star_x\end{array}$	$\underline{m}_{yz}$	$\begin{array}{l}m_{y\bar{z}}\\ \underline{m}_{yz}m_{y\bar{z}}\underline{2}^\star_x\end{array}$	AR* SI
$3_p m_{x\bar{y}}$	$m^\star_x,\,2^\star_{yz}$	$m_z\bar{3}_p m_{xy}$	$[01\bar{1}]$		$\begin{array}{l}[100]_e\\ [011]\end{array}$	(14)	$\begin{array}{l}\underline{m}^\star_x 2^\star_{yz}m_{y\bar{z}}\\ m^\star_x 2^\star_{yz}m_{y\bar{z}}\end{array}$	$\underline{m}^\star_x$	$\begin{array}{l}m^\star_x 2^\star_{yz}m_{y\bar{z}}\\ m_{y\bar{z}}\end{array}$	SI AR*
$\bar{3}_p m_{x\bar{y}}$	$m^\star_x,\,m^\star_{yz}$	$m_z\bar{3}_p m_{xy}$	$[01\bar{1}]$		$\begin{array}{l}[100]\\ [011]\end{array}$	(14)	$\begin{array}{l}\underline{m}^\star_x m^\star_{yz}m_{y\bar{z}}\\ m^\star_x\underline{m}^\star_{yz}m_{y\bar{z}}\end{array}$	$\begin{array}{l}\underline{m}^\star_x\\ \underline{m}^\star_{yz}\end{array}$	$\begin{array}{l}m^\star_x 2^\star_{yz}m_{y\bar{z}}\\ 2^\star_x\underline{m}^\star_{yz}m_{y\bar{z}}\end{array}$	SR SR

† Equations for directions of axes and shear angle φ:

$$\begin{pmatrix} a & f & e \\ f & b & d \\ e & d & c \end{pmatrix}$$
(a) [001] $[1\frac{d}{e}0]$

$$\begin{pmatrix} a & d & 0 \\ d & b & 0 \\ 0 & 0 & c \end{pmatrix}$$
(b) $[\bar{1}\alpha0]$ $[\alpha10]$

$$\alpha = \frac{2d+\sqrt{(a-b)^2+4d^2}}{a-b}$$

(c) $[\bar{1}\beta0]$ $[\beta10]$

$$\beta = \frac{(a-b)+2\sqrt{3}d+4\sqrt{(a-b)^2+4d^2}}{\sqrt{3}(a-b)-2d}$$

(1) $2\sqrt{d^2+e^2}$

(2) $2|d|$
(3) $\frac{1}{2}\sqrt{(a-b)^2+4d^2}$
(4) $\frac{\sqrt{3}}{2}\sqrt{(a-b)^2+4d^2}$

$$\begin{pmatrix} a & 0 & 0 \\ 0 & b & d \\ 0 & d & c \end{pmatrix}$$
(d) [110] $[1\bar{1}\frac{2d}{a-b}]$

(e) $[\bar{1}\sqrt{3}0]$ $[\sqrt{3}1\frac{4d}{b-a}]$

(f) $[\sqrt{3}\bar{1}0]$ $[\bar{1}\sqrt{3}\frac{4\sqrt{3}}{3(a-b)}]$

(5) $\sqrt{(a-b)^2+2d^2}$
(6) $\frac{\sqrt{3}}{2}\sqrt{(a-b)^2+4d^2}$
(7) $2|d|$

$$\begin{pmatrix} a & b & -d \\ b & a & d \\ -d & d & c \end{pmatrix}$$
(g) [100] $[0\bar{1}\frac{d}{b}]$

$$\begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix}$$
(h) [101] $[\bar{1}\frac{2d}{c-d}1]$

(8) $2\sqrt{a^2+b^2}$

(9) $\frac{\sqrt{3}}{2}|a-b|$
(10) $|a-b|$

$$\begin{pmatrix} a & d & 0 \\ d & a & 0 \\ 0 & 0 & c \end{pmatrix}$$

(11) $\sqrt{(a-c)^2+2d^2}$
(12) $2|d|$

$$\begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & c \end{pmatrix}$$
(13) $|a-c|$

$$\begin{pmatrix} a & d & d \\ d & a & d \\ d & d & a \end{pmatrix}$$
(14) $2\sqrt{2}|d|$

normals and its direction **h** is defined by a vector product $\mathbf{h} = \mathbf{n}_1 \times \mathbf{n}_2$ of normal vectors $\mathbf{n}_1$ and $\mathbf{n}_2$ of these walls. Letters B and C denote components of **h** which depend on spontaneous strain.

Equation: a reference to an expression, given at the end of the table, for the direction **h** of the axis, where parameters B and C in the column *Axis* are expressed as functions of spontaneous strain components. The matrices above these expressions give the form of the 'absolute' spontaneous strain.

Wall normals: orientation of equally deformed planes. As explained above, each plane represents two mutually reversed compatible domain walls. Numbers or parameters B, C given in parentheses can be interpreted either as components of normal

vectors to compatible walls or as intercepts analogous to Miller indices: Planes of compatible domain walls $Ax_1 + Bx_2 + Cx_3 = 0$ and $A'x_1 + B'x_2 + C'x_3 = 0$ [see equations (3.4.3.55)] pass through the origin of the Cartesian coordinate system of K_{1j} and have normal vectors $\mathbf{n}_1 = [ABC]$ and $\mathbf{n}_2 = [A'B'C']$. It is possible to find a plane with the same normal vector $[ABC]$ but not passing through the origin, *e.g.* $Ax_1 + Bx_2 + Cx_3 = 1$. Then parameters A, B and C can be interpreted as the reciprocal values of the oriented intercepts on the coordinate axes cut by this plane, $[x_1/(1/A)] + [x_2/(1/B)] + [x_3/(1/C)] = 1$. In analogy with Miller indices, the symbol (ABC) is used for expressing the orientation of a wall. However, parameters A, B and C are not Miller indices, since they are expressed in an orthonormal and

3. PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

not a crystallographic coordinate system. A left square bracket [in front of two equally deformed planes signifies that the two domain walls (domain twins) associated with one equally deformed plane are crystallographically equivalent (in K_{1j}) with two domain walls (twins) associated with the perpendicular equally deformed plane, *i.e.* all four compatible domain walls (domain twins) that can be formed from domain pair $(\mathbf{S}_1, \mathbf{S}_j)$ are crystallographically equivalent in K_{1j}.

The subscript e indicates that the wall carries a nonzero polarization charge, Div $\mathbf{P} \neq 0$. This can happen in ferroelectric domain pairs with spontaneous polarization not parallel to the axis of the pair. If one domain wall is charged then the perpendicular wall is not charged. In a few cases, polarization and/or orientation of the domain wall is not determined by symmetry; then it is not possible to specify which of the two walls is charged. In such cases, a subscript $e0$ or $0e$ indicates that one of the two walls is charged and the other is not.

φ: reference to an expression, given at the end of the table, in which the shear angle φ (in radians) is given as a function of the 'absolute' spontaneous strain components, which are defined in a matrix given above the equations.

$\bar{J}_{1j}$: symmetry of the 'twin pair'. The meaning of this group and its symbol is explained in the next section. This group specifies the symmetry properties of a ferroelastic domain twin and the reversed twin with compatible walls of a given orientation and with domain states $\mathbf{S}_1^+, \mathbf{S}_j^-$ and $\mathbf{S}_1^+, \mathbf{S}_j^-$. This group can be used for designating a twin law of the ferroelastic domain twin.

$\underline{t}_{1j}^\star$: one non-trivial twinning operation of the twin $\mathbf{S}_1[ABC]\mathbf{S}_j$ and the wall. An underlined symbol with a star symbol signifies an operation that inverts the wall normal and exchanges the domain states (see the next section).

$\bar{T}_{1j}$: layer-group symmetry of the ferroelastic domain twin and the reversed twin with compatible walls of a given orientation. Contains all trivial and non-trivial symmetry operations of the domain twin (see the next section).

Classification: symbol that specifies the type of domain twin and the wall. Five types of twins and domain walls are given in Table 3.4.4.3. The letter S denotes a symmetric domain twin (wall) in which the structures in two half-spaces are related by a symmetry operation of the twin, A denotes an asymmetric twin where there is no such relation. The letters R (reversible) and I (irreversible) signify whether a twin and reversed twin are, or are not, crystallographically equivalent in K_{1j}.

Example 3.4.3.7. **The rhombohedral phase of perovskite crystals.** Examples include PZN-PT and PMN-PT solid solutions (see *e.g.* Erhart & Cao, 2001) and BaTiO$_3$ below 183 K. The phase transition has symmetry descent $m\bar{3}m \supset 3m$.

In Table 3.4.2.7 we find that there are eight domain states and eight ferroelectric domain states. In this fully ferroelectric phase, domain states can be specified by unit vectors representing the direction of spontaneous polarization. We choose $\mathbf{S}_1 \equiv [111]$ with corresponding symmetry group $F_1 = 3_p m_{z\bar{y}}$.

From eight domain states one can form $7 \times 8 = 56$ domain pairs. These pairs can be divided into classes of equivalent pairs which are specified by different twinning groups. In column K_{1j} of Table 3.4.2.7 we find three twinning groups:

(i) The first twin law $\bar{3}_p^\star m_{x\bar{y}}$ characterizes a non-ferroelastic pair (Fam$\bar{3}_p^\star m_{x\bar{y}}$ = Fam$3_p^\star m_{x\bar{y}}$) with inversion $\bar{1}$ as a twinning operation of this pair. A representative domain pair is $(\mathbf{S}_1, g_{12}\mathbf{S}_1 = \mathbf{S}_2) = ([111], [\bar1\bar1\bar1])$, domain pairs consist of two domain states with antiparallel spontaneous polarization ('180° pairs'). Domain walls of low energy are not charged, *i.e.* they are parallel with the spontaneous polarization.

(ii) The second twinning group $K_{13} = \bar{4}3m$ characterizes a ferroelastic domain pair (Fam$\bar{4}3m = m\bar{3}m \neq$ Fam$F_1 = \bar{3}_p m_{z\bar{y}}$). In Table 3.4.3.6, we find $g_{13}^\star = 2_x^\star$, which defines the representative pair $([111], [11\bar{1}])$ ('109° pairs'). Orientations of compatible

Table 3.4.3.7. *Ferroelastic domain pairs with no compatible domain walls*

F_1 is the symmetry of $\mathbf{S}_1$, g_{1j} is the switching operation, K_{1j} is the twinning group. Pair is the domain pair type, where ns is non-transposable simple and nm is non-transposable multiple (see Table 3.4.3.2). $v = z$, $p = [111]$, $q = [\bar{1}11]$, $r = [1\bar{1}1]$, $s = [\bar{1}1\bar{1}]$ (see Table 3.4.2.5 and Fig. 3.4.2.3).

F_1	g_{1j}	K_{1j}	Pair
1	4_z	4_z	ns
1	$\bar{4}_z$	$\bar{4}_z$	ns
1	3_v	3_v	ns
1	$\bar{3}_v$	$\bar{3}_v$	ns
1	6_z	6_z	ns
1	$\bar{6}_z$	$\bar{6}_z$	ns
$\bar{1}$	$4_z, 4_z^3$	$4_z/m_z$	ns
$\bar{1}$	$3_v, 3_v^2$	$\bar{3}_v$	ns
$\bar{1}$	$6_z, 6_z^5$	$6_z/m_z$	ns
2_z	$3_p, 3_p^2$	2_z3_p	nm
2_z	$\bar{3}_p, \bar{3}_p^5$	$m_z\bar{3}_p$	nm
2_{xy}	$3_p, 3_p^2$	$4_z3_p2_{xy}$	nm
2_{xy}	$\bar{3}_p, \bar{3}_p^5$	$m_z\bar{3}_pm_{xy}$	nm
m_z	$3_p, 3_p^2$	$m_z3_p^2$	nm
m_{xy}	$3_p, 3_p^2$	$\bar{4}_z3_pm_{xy}$	nm
m_{xy}	$4_x, 4_x^3$	$m_z\bar{3}_pm_{xy}$	nm
$2_z/m_z$	$3_p, 3_p^2$	$m_z\bar{3}_p$	nm
$2_{xy}/m_{xy}$	$3_p, 3_p^2$	$m_z\bar{3}_pm_{xy}$	nm
$2_x2_y2_z$	$3_p, 3_p^2$	2_z3_p	ns
$2_x2_y2_z$	$\bar{3}_p, \bar{3}_p^5$	$m_z\bar{3}_p$	ns
$m_xm_y2_z$	$3_p, 3_p^2$	$m_z\bar{3}_p$	nm
$m_xm_ym_z$	$3_p, 3_p^2$	$m_z\bar{3}_p$	ns

domain walls of this domain pair are (100) and (011)$_e$ (this wall is charged). All equivalent orientations of these compatible walls will appear if all crystallographically equivalent pairs are considered.

(iii) The third twinning group $K_{14} = m\bar{3}m$ also represents ferroelastic domain pairs with representative pair $([111], m_x^\star[111]) = ([111], [\bar{1}11])$ ('71° pairs') and compatible wall orientations $(100)_e$ and (011). We see that for a given crystallographic orientation both charged and non-charged domain walls exist; for a given orientation the charge specifies to which class the domain wall belongs.

These conclusions are useful in deciphering the 'domain-engineered structures' of these crystals (Yin & Cao, 2000).

3.4.3.6.5. Ferroelastic domain pairs with no compatible domain walls, synoptic table

Ferroelastic domain pairs for which condition (3.4.3.54) for the existence of coherent domain walls is violated are listed in Table 3.4.3.7. All these pairs are non-transposable pairs. It is expected that domain walls between ferroelastic domain states would be stressed and would contain dislocations. Dudnik & Shuvalov (1989) have shown that in thin samples, where elastic stresses are reduced, 'almost coherent' ferroelastic domain walls may exist.

Example 3.4.3.8. **Ferroelastic crystal of langbeinite.** Langbeinite K$_2$Mg$_2$(SO$_4$)$_3$ undergoes a phase transition with symmetry descent $23 \supset 222$ that appears in Table 3.4.3.7. The ferroelastic phase has three ferroelastic domain states. Dudnik & Shuvalov (1989) found, in accord with their theoretical predictions, nearly linear 'almost coherent' domain walls accompanied by elastic stresses in crystals thinner than 0.5 mm. In thicker crystals, elastic stresses became so large that crystals were cracking and no domain walls were observed.

Similar effects were reported by the same authors for the partial ferroelastic phase of CH$_3$NH$_3$Al(SO$_4$)$_2\cdot$12H$_2$O (MASD)
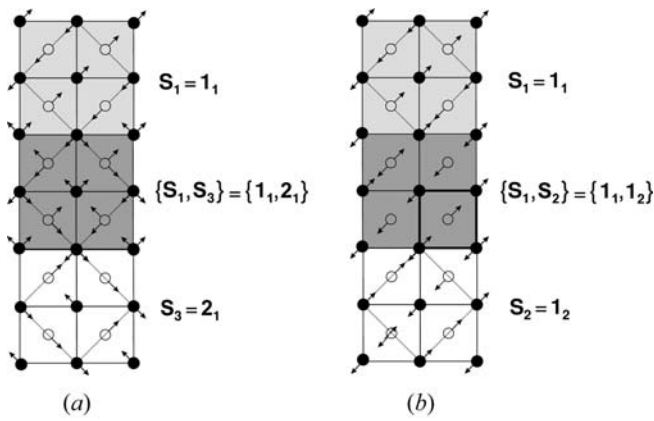
Fig. 3.4.3.10. Domain pairs in calomel. Single-domain states in the parent clamping approximation are those from Fig. 3.4.2.5. The first domain state of a domain pair is shown shaded in grey ('black'), the second domain state is colourless ('white'), and the domain pair of two interpenetrating domain states is shown shaded in dark grey. (a) Ferroelastic domain pair (S_1, S_3) in the parent clamping approximation. This is a partially transposable domain pair. (b) Translational domain pair (S_1, S_2). This is a completely transposable domain pair.

with symmetry descent $\bar{3}m \supset mmm$, where ferroelastic domain walls were detected only in thin samples.

3.4.3.7. Domain pairs in the microscopic description

In the *microscopic description*, two microscopic domain states S_i and S_k with space-group symmetries $\mathcal{F}_i$ and $\mathcal{F}_k$, respectively, can form an ordered domain pair (S_i, S_k) and an unordered domain pair $\{S_i, S_k\}$ in a similar way to in the continuum description, but one additional aspect has to be considered. The definition of the symmetry group $\mathcal{F}_{ik}$ of an ordered domain pair (S_i, S_k),

$$\mathcal{F}_{ik} = \mathcal{F}_i \cap \mathcal{F}_k, \qquad (3.4.3.72)$$

is meaningful only if the group $\mathcal{F}_{ik}$ is a space group with a three-dimensional translational subgroup (three-dimensional *twin lattice* in the classical description of twinning, see Section 3.3.8)

$$\mathcal{T}_{ik} = \mathcal{T}_i \cap \mathcal{T}_k, \qquad (3.4.3.73)$$

where $\mathcal{T}_i$ and $\mathcal{T}_k$ are translation subgroups of $\mathcal{F}_i$ and $\mathcal{F}_k$, respectively. This condition is fulfilled if both domain states S_i and S_k have the same spontaneous strains, *i.e.* in non-ferroelastic domain pairs, but in ferroelastic domain pairs one has to suppress spontaneous deformations by applying the parent clamping approximation [see Section 3.4.2.2, equation (3.4.2.49)].

Example 3.4.3.9. Domain pairs in calomel. Calomel undergoes a non-equitranslational phase transition from a tetragonal parent phase to an orthorhombic ferroelastic phase (see Example 3.4.2.7 in Section 3.4.2.5). Four basic microscopic single-domain states are displayed in Fig. 3.4.2.5. From these states, one can form 12 non-trivial ordered single-domain pairs that can be partitioned (by means of double coset decomposition) into two orbits of domain pairs.

Representative domain pairs of these orbits are depicted in Fig. 3.4.3.10, where the first microscopic domain state S_i participating in a domain pair is displayed in the upper cell (light grey) and the second domain state S_j, $j = 2, 3$, in the lower white cell. The overlapping structure in the middle (dark grey) is a geometrical representation of the domain pair $\{S_i, S_j\}$.

The domain pair $\{S_1, S_3\}$, depicted in Fig. 3.4.3.10(a), is a ferroelastic domain pair in the parent clamping approximation. Then two overlapping structures of the domain pair have a common three-dimensional lattice with a common unit cell (the
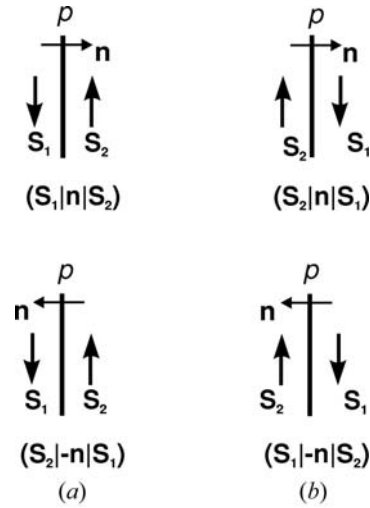

Fig. 3.4.4.1. Symbols of a simple twin. (a) Two different symbols with antiparallel normal **n**. (b) Symbols of the reversed twin.

dotted square), which is the same as the unit cells of domain states S_1 and S_3.

Domain pair $\{S_1, S_2\}$, shown in Fig. 3.4.3.10(b), is a translational (antiphase) domain pair in which domain states S_1 and S_2 differ only in location but not in orientation. The unit cell (heavily outlined small square) of the domain pair $\{S_1, S_2\}$ is identical with the unit cell of the tetragonal parent phase (*cf.* Fig. 3.4.2.5).

The two arrows attached to the circles in the domain pairs represent exaggerated displacements within the wall.

Domain pairs represent an intermediate step in analyzing microscopic structures of domain walls, as we shall see in Section 3.4.4.

3.4.4. Domain twins and domain walls

3.4.4.1. Formal description of simple domain twins and planar domain walls of zero thickness

In this section, we examine crystallographic properties of planar compatible domain walls and simple domain twins. The symmetry of these objects is described by layer groups. Since this concept is not yet common in crystallography, we briefly explain its meaning in Section 3.4.4.2. The exposition is performed in the continuum description, but most of the results apply with slight generalizations to the microscopic treatment that is illustrated with an example in Section 3.4.4.7.

We shall consider a *simple domain twin* T_{12} that consists of two domains D_1 and D_2 which meet along a planar domain wall W_{12} of zero thickness. Let us denote by p a *plane of the domain wall*, in brief *wall plane* of W_{12}. This plane is specified by Miller indices (hkl), or by a normal **n** to the plane which also defines the sidedness (plus and minus side) of the plane p. By *orientation of the plane p* we shall understand a specification which can, but may not, include the sidedness of p. If both the orientation and the sidedness are given, then the plane p divides the space into two half-spaces. Using the bra–ket symbols, mentioned in Section 3.4.3.6, we shall denote by (| the half-space on the negative side of p and by |) the half-space on the positive side of p.

A *simple twin* consists of two (theoretically semi-infinite) domains D_1 and D_2 with domain states S_1 and S_2, respectively, that join along a planar domain wall the orientation of which is specified by the wall plane p with normal **n**. A symbol $(S_1|n|S_2)$ specifies the domain twin unequivocally: domain $(S_1|$, with domain region (| filled with domain state S_1, is on the negative side of p and domain $|S_2)$ is on the positive side of p (see Fig. 3.4.4.1a).