International Tables for Crystallography (2013). Vol. D, Section 3.4.3.2, pp. 508–510.

The star in the symbol $J^{\star}_{ik}$ 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 $g^{\star}_{ik}F_i$ 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

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

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 $G = 4_z/m_zm_xm_{xy} \supset 2_xm_ym_z = F_1$ 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

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

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

$$J^{\star}_{12} = 2_xm_ym_z \cup m^{\star}_x\{2_xm_ym_z\} = m^{\star}_xm_ym_z. \qquad (3.4.3.18)$$

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:

$$F_{13} = F_1 \cap F_3 = 2_xm_ym_z \cap m_x2_ym_z = \{1, m_z\} \equiv \{m_z\}, \qquad (3.4.3.19)$$

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; 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 $g^{\star}_{1j}F_1$ forms a group that is identical with the symmetry group $J^{\star}_{1j}$ of the unordered domain pair $\{\mathbf{S}_1, \mathbf{S}_j\}$:

$$K^{\star}_{1j} = J^{\star}_{1j} = F_1 \cup g^{\star}_{1j}F_1, \quad g^{\star}_{1j} \in K_{1j}, \quad F_1 = F_j. \qquad (3.4.3.24)$$

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,

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

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),

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

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 $K_{1j} \supset F_1$,

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

where $\kappa^{(1)}_a$ and $\kappa^{(j)}_a$ 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 $\kappa^{(1)}_a$ 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 $(\mathbf{S}_1, \mathbf{S}_j)$,

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

[*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:

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

where $\lambda^{(1)}_b$ and $\lambda^{(j)}_b$ are the secondary tensor parameters in domain states $\mathbf{S}_1$ and $\mathbf{S}_j$; the last equation, in which $I_{K_{1j}}(\lambda^{(1)}_b)$ is the stabilizer of $\lambda^{(1)}_b$ 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 $\lambda^{(1)}_b$ 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 $\lambda^{(j)}_b$ in domain state $\mathbf{S}_j$ can be obtained by applying to the secondary tensor parameters $\lambda^{(1)}_b$ 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),

$$K^{\star}_{12} = J^{\star}_{12} = 2_x m_y m_z \cup m^{\star}_x\{2_x m_y m_z\} = m^{\star}_x m_y m_z. \qquad (3.4.3.30)$$

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 $g^{\star}_{12}$ is for example the inversion $\bar{1}$, the tensor parameter $\kappa^{(2)}_1$ in the second domain state $\mathbf{S}_2$ is $\kappa^{(2)}_1 = -P_1$.

Other principal tensor parameters can be found in the software *GI⋆KoBo*-1 or in Kopský (2001), p. 185. They are: $\kappa^{(1)}_2 = d_{12}$, $\kappa^{(1)}_3 = d_{13}$, $\kappa^{(1)}_4 = d_{26}$, $\kappa^{(1)}_5 = d_{35}$ (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

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

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 $\kappa^{(3)}_1 = D(2_{xy})(P, 0) = (0, P)$. 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: $\lambda_1^{(1)} = u_1 - u_2$; $\lambda_2^{(1)} = A_{14} + A_{25}, A_{36}$; $\lambda_3^{(1)} = s_{11} - s_{22}$, $s_{13} - s_{23}$, $s_{44} - s_{55}$; $\lambda_4^{(1)} = Q_{11} - Q_{22}$, $Q_{12} - Q_{21}$, $Q_{13} - Q_{23}$, $Q_{31} - Q_{32}$, $Q_{44} - Q_{55}$. 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)

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

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

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

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

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	$\sigma\sigma$
...	...	...	...	...

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

references