International Tables for Crystallography (2013). Vol. D, Section 3.4.3.5, pp. 512–515.

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	$\bar{3}_z^5$	$\bar{6}_z$	$\mathbf{S}_3$

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, $(\mathbf{S}_1, 2_{xy}\mathbf{S}_1) = (\mathbf{S}_1, \mathbf{S}_3)$ 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

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 $K_{1j}^\star$; ρ, $P_i, \ldots, Q_{\mu\nu}$: components of property tensors (see Table 3.4.3.5): $a|c$: number of distinct|equal nonzero independent tensor components of property tensors.

F_1	$g_{1j}^\star$	$K_{1j}^\star = J_{1j}^\star$	Γ_α	Diffraction intensities	ρ	P_i	g_μ	$d_{i\mu}$	$A_{i\mu}$	$s_{\mu\nu}$	$Q_{\mu\nu}$
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
$m_xm_y2_z$	$\bar{1}^\star$, $m_z^\star$, $2_x^\star$, $2_y^\star$	$m_xm_ym_z^\star$	B_{1u}	=	0|0	1|0	1|0	5|0	0|3	0|9	0|12
$2_xm_ym_z$	$\bar{1}^\star$, $m_x^\star$, $2_y^\star$, $2_z^\star$	$m_x^\star m_ym_z$	B_{1u}	=	0|0	1|0	1|0	5|0	0|3	0|9	0|12
$m_x2_ym_z$	$\bar{1}^\star$, $m_y^\star$, $2_x^\star$, $2_z^\star$	$m_xm_y^\star m_z$	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	$2_x^\star$, $2_y^\star$, $2_{xy}^\star$, $2_{x\bar{y}}^\star$	$4_z2_x^\star 2_{xy}^\star$	A_2	≠	0|1	1|0	0|2	3|1	3|1	1|6	3|7
4_z	$m_x^\star$, $m_y^\star$, $m_{xy}^\star$, $m_{x\bar{y}}^\star$	$4_zm_x^\star m_{xy}^\star$	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
$\bar{4}_z$	$m_{xy}^\star$, $m_{x\bar{y}}^\star$, $2_x^\star$, $2_y^\star$	$\bar{4}_z2_x^\star m_{xy}^\star$	A_2	≠	0|0	0|0	1|1	2|2	3|1	1|6	3|7
$\bar{4}_z$	$m_x^\star$, $m_y^\star$, $2_{xy}^\star$, $2_{x\bar{y}}^\star$	$\bar{4}_zm_x^\star 2_{xy}^\star$	A_2	≠	0|0	0|0	1|1	2|2	3|1	1|6	3|7
$4_z/m_z$	$m_x^\star$, $m_y^\star$, $m_{xy}^\star$, $m_{x\bar{y}}^\star$, $2_x^\star$, $2_y^\star$, $2_{xy}^\star$, $2_{x\bar{y}}^\star$	$4_z/m_zm_x^\star m_{xy}^\star$	A_{2g}	≠	0|0	0|0	0|0	0|0	3|1	1|6	3|7
$4_z2_x2_{xy}$	$\bar{1}^\star$, $m_z^\star$, $m_x^\star$, $m_y^\star$, $m_{xy}^\star$, $m_{x\bar{y}}^\star$	$4_z/m_z^\star m_x^\star m_{xy}^\star$	A_{1u}	=	1|0	0|0	2|0	1|0	0|1	0|6	0|7
$4_zm_xm_{xy}$	$\bar{1}^\star$, $m_z^\star$, $2_x^\star$, $2_y^\star$, $2_{xy}^\star$, $2_{x\bar{y}}^\star$	$4_z/m_z^\star m_xm_{xy}$	A_{2u}	=	0|0	1|0	0|0	3|0	0|1	0|6	0|7
$\bar{4}_z2_xm_{xy}$	$\bar{1}^\star$, $m_z^\star$, $m_x^\star$, $m_y^\star$, $2_{xy}^\star$, $2_{x\bar{y}}^\star$	$4_z^\star/m_z^\star m_x^\star m_{xy}$	B_{1u}	=	0|0	0|0	1|0	2|0	0|1	0|6	0|7
$\bar{4}_zm_x2_{xy}$	$\bar{1}^\star$, $m_z^\star$, $m_{xy}^\star$, $m_{x\bar{y}}^\star$, $2_x^\star$, $2_y^\star$	$4_z^\star/m_z^\star m_xm_{xy}^\star$	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	$2_x^\star$, $2_{x'}^\star$, $2_{x''}^\star$	$3_z2_x^\star$	A_2	≠	0|1	1|0	0|2	4|2	4|2	1|6	4|8
3_z	$2_y^\star$, $2_{y'}^\star$, $2_{y''}^\star$	$3_z2_y^\star$	A_2	≠	0|1	1|0	0|2	4|2	4|2	1|6	4|8
3_p	$2_{x\bar{y}}^\star$, $2_{y\bar{z}}^\star$, $2_{z\bar{x}}^\star$	$3_p2_{x\bar{y}}^\star$	A_2	≠	0|1	1|0	0|2	4|2	4|2	1|6	4|8
3_z	$m_x^\star$, $m_{x'}^\star$, $m_{x''}^\star$	$3_zm_x^\star$	A_2	≠	1|0	0|1	2|0	2|4	4|2	1|6	4|8
3_z	$m_y^\star$, $m_{y'}^\star$, $m_{y''}^\star$	$3_zm_y^\star$	A_2	≠	1|0	0|1	2|0	2|4	4|2	1|6	4|8
3_p	$m_{x\bar{y}}^\star$, $m_{y\bar{z}}^\star$, $m_{z\bar{x}}^\star$	$3_pm_x^\star$	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
$\bar{3}_z$	$m_x^\star$, $m_{x'}^\star$, $m_{x''}^\star$, $2_x^\star$, $2_{x'}^\star$, $2_{x''}^\star$	$\bar{3}_zm_x^\star$	A_{2g}	≠	0|0	0|0	0|0	0|0	4|2	1|6	4|8
$\bar{3}_z$	$m_y^\star$, $m_{y'}^\star$, $m_{y''}^\star$, $2_y^\star$, $2_{y'}^\star$, $2_{y''}^\star$	$\bar{3}_zm_y^\star$	A_{2g}	≠	0|0	0|0	0|0	0|0	4|2	1|6	4|8
$\bar{3}_p$	$m_{x\bar{y}}^\star$, $m_{y\bar{z}}^\star$, $m_{z\bar{x}}^\star$, $2_{x\bar{y}}^\star$, $2_{y\bar{z}}^\star$, $2_{z\bar{x}}^\star$	$\bar{3}_pm_x^\star$	A_{2g}	≠	0|0	0|0	0|0	0|0	4|2	1|6	4|8
$\bar{3}_z$	$m_z^\star$, $2_z^\star$	$6_z^\star/m_z^\star$	B_g	≠	0|0	0|0	0|0	0|0	2|4	2|5	4|8
3_z2_x	$\bar{1}^\star$, $m_x^\star$, $m_{x'}^\star$, $m_{x''}^\star$	$\bar{3}_z^\star m_x^\star$	A_{1u}	=	1|0	0|0	2|0	2|0	0|2	0|6	0|8
3_z2_y	$\bar{1}^\star$, $m_y^\star$, $m_{y'}^\star$, $m_{y''}^\star$	$\bar{3}_z^\star m_y^\star$	A_{1u}	=	1|0	0|0	2|0	2|0	0|2	0|6	0|8
3_z2_x	$2_z^\star$, $2_y^\star$, $2_{y'}^\star$, $2_{y''}^\star$	$6_z^\star 2_x2_y^\star$	B_1	≠	0|1	0|0	0|2	1|1	1|1	1|5	2|6
3_z2_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
$3_p2_{x\bar{y}}$	$\bar{1}^\star$, $m_{x\bar{y}}^\star$, $m_{y\bar{z}}^\star$, $m_{z\bar{x}}^\star$	$\bar{3}_p^\star m_x^\star$	A_{1u}	=	1|0	0|0	2|0	2|0	0|2	0|6	0|8
3_z2_x	$m_z^\star$, $m_y^\star$, $m_{y'}^\star$, $m_{y''}^\star$	$\bar{6}_z^\star 2_xm_y^\star$	A_1''	≠	1|0	0|0	2|0	1|1	1|1	1|5	2|6
3_z2_y	$m_z^\star$, $m_x^\star$, $m_{x'}^\star$, $m_{x''}^\star$	$\bar{6}_z^\star m_x2_y^\star$	A_1''	≠	1|0	0|0	2|0	1|1	1|1	1|5	2|6
$3_pm_{x\bar{y}}$	$\bar{1}^\star$, $2_{x\bar{y}}^\star$, $2_{y\bar{z}}^\star$, $2_{z\bar{x}}^\star$	$\bar{3}_p^\star m_x$	A_{2u}	=	0|0	1|0	0|0	4|0	0|2	0|6	0|8
3_zm_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_zm_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_zm_x	$2_z^\star$, $m_y^\star$, $m_{y'}^\star$, $m_{y''}^\star$	$6_z^\star m_xm_y^\star$	B_2	≠	0|0	0|1	0|0	1|3	1|1	1|5	2|6
3_zm_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_zm_x	$m_z^\star$, $2_y^\star$, $2_{y'}^\star$, $2_{y''}^\star$	$\bar{6}_z^\star m_x2_y^\star$	A_2''	≠	0|0	1|0	0|0	3|1	1|1	1|5	2|6
3_zm_y	$m_z^\star$, $2_x^\star$, $2_{x'}^\star$, $2_{x''}^\star$	$\bar{6}_z^\star 2_x^\star m_y$	A_2''	≠	0|0	1|0	0|0	3|1	1|1	1|5	2|6
$\bar{3}_zm_x$	$m_z^\star$, $m_y^\star$, $m_{y'}^\star$, $m_{y''}^\star$	$6_z^\star/m_z^\star m_xm_y^\star$	B_{1g}	≠	0|0	0|0	0|0	0|0	1|1	1|5	2|6
$\bar{3}_zm_y$	$m_z^\star$, $m_x^\star$, $m_{x'}^\star$, $m_{x''}^\star$	$6_z^\star/m_z^\star m_x^\star m_y$	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	$2_x^\star$, $2_{x'}^\star$, $2_{x''}^\star$, $2_y^\star$, $2_{y'}^\star$, $2_{y''}^\star$	$6_z2_x^\star 2_y^\star$	A_2	≠	0|1	1|0	0|2	3|1	3|1	0|5	2|6
6_z	$m_x^\star$, $m_{x'}^\star$, $m_{x''}^\star$, $m_y^\star$, $m_{y'}^\star$, $m_{y''}^\star$	$6_zm_x^\star m_y^\star$	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
$\bar{6}_z$	$m_x^\star$, $m_{x'}^\star$, $m_{x''}^\star$, $2_y^\star$, $2_{y'}^\star$, $2_{y''}^\star$	$\bar{6}_zm_x^\star 2_y^\star$	A_2'	≠	0|0	0|0	0|0	1|1	3|1	0|5	2|6
$\bar{6}_z$	$m_y^\star$, $m_{y'}^\star$, $m_{y''}^\star$, $2_x^\star$, $2_{x'}^\star$, $2_{x''}^\star$	$\bar{6}_z2_x^\star m_y^\star$	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	ρ	P_i	g_μ	$d_{i\mu}$	$A_{i\mu}$	$s_{\mu\nu}$	$Q_{\mu\nu}$
$6_z/m_z$	$m^\star_x, m^\star_{x'}, m^\star_{x''}, m^\star_y, m^\star_{y'}, m^\star_{y''}, 2^\star_x, 2^\star_{x'}, 2^\star_{x''}, 2^\star_y, 2^\star_{y'}, 2^\star_{y''}$	$6_z/m_z m^\star_x m^\star_y$	A_{2g}	$\neq$	0|0	0|0	0|0	0|0	3|1	0|5	2|6
$6_z 2_x 2_y$	$\bar{1}^\star, m^\star_z, m^\star_x, m^\star_{x'}, m^\star_{x''}, m^\star_y, m^\star_{y'}, m^\star_{y''}$	$6_z/m^\star_z m^\star_x m^\star_y$	A_{1u}	=	1|0	0|0	2|0	1|0	0|1	0|5	0|6
$6_z m_x m_y$	$\bar{1}^\star, m^\star_z, 2^\star_x, 2^\star_{x'}, 2^\star_{x''}, 2^\star_y, 2^\star_{y'}, 2^\star_{y''}$	$6_z/m^\star_z m_x m_y$	A_{2u}	=	0|0	1|0	0|0	3|0	0|1	0|5	0|6
$\bar{6}_z 2_x m_y$	$\bar{1}^\star, 2^\star_z, m^\star_x, m^\star_{x'}, m^\star_{x''}, 2^\star_y, 2^\star_{y'}, 2^\star_{y''}$	$6^\star_z/m_z m^\star_x m_y$	B_{2u}	=	0|0	0|0	0|0	1|0	0|1	0|5	0|6
$\bar{6}_z m_x 2_y$	$\bar{1}^\star, 2^\star_z, m^\star_y, m^\star_{y'}, m^\star_{y''}, 2^\star_x, 2^\star_{x'}, 2^\star_{x''}$	$6^\star_z/m_z m_x m^\star_y$	B_{2u}	=	0|0	0|0	0|0	1|0	0|1	0|5	0|6
23	$\bar{1}^\star, m^\star_x, m^\star_y, m^\star_z$	$m^\star\bar{3}$	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	$m^\star_{xy}, m^\star_{yz}, m^\star_{zx}, m^\star_{x\bar{y}}, m^\star_{y\bar{z}}, m^\star_{z\bar{x}}$	$\bar{4}^\star 3m^\star$	A_2	$\neq$	1|0	0|0	1|0	0|1	1|0	0|3	1|3
$m\bar{3}$	$m^\star_{xy}, m^\star_{yz}, m^\star_{zx}, m^\star_{x\bar{y}}, m^\star_{y\bar{z}}, m^\star_{z\bar{x}}, 2^\star_{xy}, 2^\star_{yz}, 2^\star_{zx}, 2^\star_{x\bar{y}}, 2^\star_{y\bar{z}}, 2^\star_{z\bar{x}}$	$m\bar{3}m^\star$	A_{2g}	$\neq$	0|0	0|0	0|0	0|0	1|0	0|3	1|3
432	$\bar{1}^\star, m^\star_x, m^\star_y, m^\star_z, m^\star_{xy}, m^\star_{yz}, m^\star_{zx}, m^\star_{x\bar{y}}, m^\star_{y\bar{z}}, m^\star_{z\bar{x}}$	$m^\star\bar{3}m^\star$	A_{1u}	=	1|0	0|0	1|0	0|0	0|0	0|3	0|3
$\bar{4}3m$	$\bar{1}^\star, m^\star_x, m^\star_y, m^\star_z, 2^\star_{xy}, 2^\star_{yz}, 2^\star_{zx}, 2^\star_{x\bar{y}}, 2^\star_{y\bar{z}}, 2^\star_{z\bar{x}}$	$m^\star\bar{3}m$	A_{2u}	=	0|0	0|0	0|0	1|0	0|0	0|3	0|3

and y; diagonal directions are abbreviated: $p = [111]$, $q = [\bar{1}\bar{1}1]$, $r = [1\bar{1}\bar{1}]$, $s = [\bar{1}1\bar{1}]$ (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.

$K^\star_{1j} = J^\star_{1j}$: *twinning group of the domain pair* $(\mathbf{S}_1, \mathbf{S}_j)$. This group is equal to the symmetry group $J^\star_{1j}$ 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 $K^\star_{1j} = J^\star_{1j}$ designates the *twin law of the non-ferroelastic domain pair* $\{\mathbf{S}_1, \mathbf{S}_j\}$ and the *twin law of all 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 (2004)].

ρ, P_i, $g_\mu, \ldots,$ $Q_{\mu\nu}$: 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.

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

Table 3.4.3.5. *Property tensors and switching fields*

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

Table 3.4.3.4		Other properties		Switching field
Component	Property tensor	Component	Property tensor	
ρ	Enantiomorphism	ρ	Optical rotatory power	
$\mathbf{P}_i$	Polarization	$\mathbf{p}_i$	Pyroelectricity	$\mathbf{E}$
ε_{ij}	Permittivity			$\mathbf{EE}$
$\mathbf{u}_\mu$	Strain			$\boldsymbol{\sigma}$
σ_μ	Mechanical stress			
g_μ	Optical activity			
$\mathbf{d}_{i\mu}$	Piezoelectricity	$\mathbf{r}_{ijk}$	Electro-optics	$\mathbf{E}\boldsymbol{\sigma}$
$A_{i\mu}$	Electrogyration			
$\mathbf{s}_{\mu\nu}$	Elastic compliance	$\mathbf{c}_{\mu\nu}$	Elastic stiffness	$\boldsymbol{\sigma\sigma}$
$\mathbf{Q}_{\mu\nu}$†	Electrostriction	$\boldsymbol{\pi}_{\mu\nu}$†	Piezo-optics	$\mathbf{EE}\boldsymbol{\sigma}$

† For contracted notation, see Section 1.1.4.10.5.

$a \neq 0$, 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 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★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 $G = \bar{6} \supset 3 = F_1$ 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 $G(= K_{1j}) = \bar{6}$ 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 $\mathbf{E} = (0, 0, E_z)$.

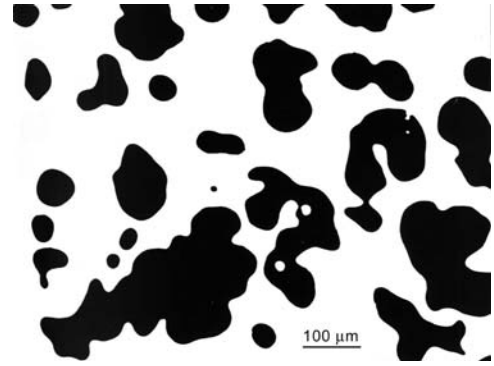

Fig. 3.4.3.3. Domain structure in lead germanate observed using a polarized-light microscope. Visualization based on the opposite sign of the optical activity coefficient in the two domain states. Courtesy of Vl. Shur, Ural State University, Ekaterinburg.

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★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 (2004)], 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 $K^\star_{12} = 6_z2_x2_z$. 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

references