

3.4. DOMAIN STRUCTURES

Table 3.4.3.4 (cont.)

F_1	g_{ij}^*	$K_{ij}^* = J_{ij}^*$	Γ_α	Diffraction intensities	ϵ	P_i	g_μ	$d_{i\mu}$	$A_{i\mu}$	$s_{\mu\nu}$	$Q_{ij\mu}$
$6_z/m_z$	$m_x^*, m_x^*, m_{x'}^*, m_y^*, m_y^*, m_{y'}^*, 2_x^*, 2_x^*, 2_{x'}^*, 2_y^*, 2_y^*, 2_{y'}^*$	$6_z/m_z m_x^* m_y^*$	A_{2g}	\neq	0 0	0 0	0 0	0 0	3 1	0 5	2 6
$6_z 2_x 2_y$	$\bar{1}^*, m_x^*, m_x^*, m_x^*, m_{x'}^*, m_y^*, m_y^*, m_{y'}^*$	$6_z/m_z m_x^* m_y^*$	A_{1u}	$=$	1 0	0 0	2 0	1 0	0 1	0 5	0 6
$6_z m_x m_y$	$\bar{1}^*, m_x^*, 2_x^*, 2_{x'}^*, 2_y^*, 2_{y'}^*, 2_{y'}^*$	$6_z/m_z m_x m_y$	A_{2u}	$=$	0 0	1 0	0 0	3 0	0 1	0 5	0 6
$\bar{6}_z 2_x m_y$	$\bar{1}^*, 2_x^*, m_x^*, m_x^*, m_{x'}^*, 2_y^*, 2_{y'}^*, 2_{y'}^*$	$6_z/m_z m_x^* m_y^*$	B_{2u}	$=$	0 0	0 0	0 0	1 0	0 1	0 5	0 6
$\bar{6}_z m_x 2_y$	$\bar{1}^*, 2_x^*, m_y^*, m_y^*, m_{y'}^*, 2_x^*, 2_{x'}^*, 2_{x'}^*$	$6_z/m_z m_x m_y^*$	B_{2u}	$=$	0 0	0 0	0 0	1 0	0 1	0 5	0 6
23	$\bar{1}^*, m_x^*, m_y^*, m_z^*$	$m^* \bar{3}$	A_u	$=$	1 0	0 0	1 0	1 0	0 1	0 3	0 4
23	$2_{xy}^*, 2_{yz}^*, 2_{zx}^*, 2_{x'y'}^*, 2_{y'z'}^*, 2_{z'x'}^*$	$4^* 32^*$	A_2	\neq	0 1	0 0	0 1	1 0	1 0	0 3	1 3
23	$m_{xy}^*, m_{yz}^*, m_{zx}^*, m_{x'y'}^*, m_{y'z'}^*, m_{z'x'}^*$	$\bar{4}^* 3m^*$	A_2	\neq	1 0	0 0	1 0	0 1	1 0	0 3	1 3
$m\bar{3}$	$m_{xy}^*, m_{yz}^*, m_{zx}^*, m_{x'y'}^*, m_{y'z'}^*, m_{z'x'}^*, 2_{xy}^*, 2_{yz}^*, 2_{zx}^*, 2_{x'y'}^*, 2_{y'z'}^*, 2_{z'x'}^*$	$m\bar{3}m^*$	A_{2g}	\neq	0 0	0 0	0 0	0 0	1 0	0 3	1 3
432	$\bar{1}^*, m_x^*, m_x^*, m_x^*, m_{xy}^*, m_{yz}^*, m_{zx}^*, m_{x'y'}^*, m_{y'z'}^*, m_{z'x'}^*$	$m^* \bar{3}m^*$	A_{1u}	$=$	1 0	0 0	1 0	0 0	0 0	0 3	0 3
$\bar{4}3m$	$\bar{1}^*, m_x^*, m_y^*, m_z^*, 2_{xy}^*, 2_{yz}^*, 2_{zx}^*, 2_{x'y'}^*, 2_{y'z'}^*, 2_{z'x'}^*$	$m^* \bar{3}m$	A_{2u}	$=$	0 0	0 0	0 0	1 0	0 0	0 3	0 3

non-ferroelastic twins with domains containing S_1 and 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 $(S_1, S_j) = (S_1, g_{ij}^* S_1)$.

Γ_α : irreducible representation of K_{ij} that defines the transformation properties of the principal tensor parameters of the symmetry descent $K_{ij} \supset F_1$ 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_{ij} .

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 intensities per unit volume of the two domain states are different [for more details, see Chapter 3.3; Catti & Ferraris (1976); Koch (1999)].

$\epsilon, P_i, g_\mu, \dots, Q_{ij\mu}$: 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 S_1 and 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 (S_1, S_j) . These tensor components are already nonzero in the parent phase.

Table 3.4.3.5. *Property tensors and switching fields*

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

Symbol	Property tensor	Symbol	Property tensor	Switching fields
ϵ	Enantiomorphism			
P_i	Polarization	p_i	Chirality	E
ϵ_{ij}	Permittivity		Pyroelectricity	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 S_1 and $S_j = g_{ij}^* S_1$. Principal tensor parameters for symmetry descents $K_{ij} \supset F_1$ 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_{ij} .

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 property 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 S_1 and 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 (S_1, S_j) differ in principal tensor parameters of the transition $K_{ij} \supset F_1$. These principal tensor parameters are Cartesian tensor