

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

Table 3.4.3.4 (cont.)

F_1	g_{1j}^*	$K_{1j}^* = J_{1j}^*$	Γ_α	Diffraction intensities	ρ	P_i	g_μ	$d_{i\mu}$	$A_{i\mu}$	$s_{\mu\nu}$	$Q_{\mu\nu}$
$6_z/m_z$	$m_x^*, m_x', m_{xy}^*, m_{xy}', m_y^*, m_y', m_{yz}^*, m_{yz}', m_z^*, m_z', m_{zx}^*, m_{zx}', m_{xy}^*, m_{xy}', m_y^*, m_y', m_{yz}^*, m_{yz}', m_z^*, m_z', m_{zx}^*, m_{zx}'$	$6_z/m_z m_x^* m_y^*$	A_{2g}	\neq	0 0	0 0	0 0	0 0	3 1	0 5	2 6
$6_z 2_x 2_y$	$\bar{1}^*, m_x^*, m_x', m_{xy}^*, m_{xy}', m_y^*, m_y', m_{yz}^*, m_{yz}', m_z^*, m_z', m_{zx}^*, m_{zx}'$	$6_z/m_x^* m_y^* m_z^*$	A_{1u}	$=$	1 0	0 0	2 0	1 0	0 1	0 5	0 6
$6_z m_x m_y$	$\bar{1}^*, m_x^*, m_x', m_{xy}^*, m_{xy}', m_y^*, m_y', m_{yz}^*, m_{yz}', m_z^*, m_z', m_{zx}^*, m_{zx}'$	$6_z/m_x^* m_y^* m_z^*$	A_{2u}	$=$	0 0	1 0	0 0	3 0	0 1	0 5	0 6
$\bar{6}_z 2_x m_y$	$\bar{1}^*, m_x^*, m_x', m_{xy}^*, m_{xy}', m_y^*, m_y', m_{yz}^*, m_{yz}', m_z^*, m_z', m_{zx}^*, m_{zx}'$	$6_z/m_x^* m_y^* m_z^*$	B_{2u}	$=$	0 0	0 0	0 0	1 0	0 1	0 5	0 6
$\bar{6}_z m_x 2_y$	$\bar{1}^*, m_x^*, m_x', m_{xy}^*, m_{xy}', m_y^*, m_y', m_{yz}^*, m_{yz}', m_z^*, m_z', m_{zx}^*, m_{zx}'$	$6_z/m_x^* m_y^* m_z^*$	B_{2u}	$=$	0 0	0 0	0 0	1 0	0 1	0 5	0 6
23	$\bar{1}^*, m_x^*, m_x', m_y^*, m_y'$	$m^* \bar{3}$	A_u	$=$	1 0	0 0	1 0	1 0	0 1	0 3	0 4
23	$2_{xy}^*, 2_{yz}^*, 2_{zx}^*, 2_{xy}^*, 2_{yz}^*, 2_{zx}^*$	$4^* 32^*$	A_2	\neq	0 1	0 0	0 1	1 0	1 0	0 3	1 3
23	$m_x^*, m_x', m_{yz}^*, m_{yz}', m_{zx}^*, m_{zx}', m_{xy}^*, m_{xy}'$	$4^* 3m^*$	A_2	\neq	1 0	0 0	1 0	0 1	1 0	0 3	1 3
$m\bar{3}$	$m_x^*, m_x', m_{yz}^*, m_{yz}', m_{zx}^*, m_{zx}', m_{xy}^*, m_{xy}', m_{yz}^*, m_{yz}', m_{zx}^*, m_{zx}', m_{xy}^*, m_{xy}'$	$m\bar{3}m^*$	A_{2g}	\neq	0 0	0 0	0 0	0 0	1 0	0 3	1 3
432	$\bar{1}^*, m_x^*, m_x', m_y^*, m_y', m_{yz}^*, m_{yz}', m_{zx}^*, m_{zx}', m_{xy}^*, m_{xy}'$	$m^* \bar{3}m^*$	A_{1u}	$=$	1 0	0 0	1 0	0 0	0 0	0 3	0 3
43m	$\bar{1}^*, m_x^*, m_x', m_y^*, m_y', m_{yz}^*, m_{yz}', m_{zx}^*, m_{zx}', m_{xy}^*, m_{xy}'$	$m^* \bar{3}m$	A_{2u}	$=$	0 0	0 0	0 0	1 0	0 0	0 3	0 3

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

$K_{1j}^* = J_{1j}^*$: twinning group of the domain pair (S_1, S_j). This group is equal to the symmetry group J_{1j}^* of the completely transposable unordered domain pair $\{S_1, S_j\}$ [see equation (3.4.3.24)]. The dichromatic symbol of the group $K_{1j}^* = J_{1j}^*$ designates the twin law of the non-ferroelastic domain pair $\{S_1, S_j\}$ and the twin law of all 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 $(S_1, S_j) = (S_1, g_{1j}^* S_1)$.

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 intensities per unit volume of the two domain states are different [for more details, see Chapter 3.3; Catti & Ferraris (1976); Koch (2004)].

$\rho, P_i, g_\mu, \dots, Q_{\mu\nu}$: 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 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.

The principal tensor parameters are one-dimensional and have the same absolute value but opposite sign in S_1 and $S_j = g_{1j}^* S_1$. 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 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

Table 3.4.3.5. Property tensors and switching fields

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

Table 3.4.3.4		Other properties		Switching field
Component	Property tensor	Component	Property tensor	
ρ	Enantiomorphism	ρ	Optical rotatory power	E
P_i	Polarization	P_i	Pyroelectricity	
ϵ_{ij}	Permittivity			EE
u_μ	Strain			σ
σ_μ	Mechanical stress			E σ
g_μ	Optical activity			
$d_{i\mu}$	Piezoelectricity	r_{ijk}	Electro-optics	E σ
$A_{i\mu}$	Electrogyration			
$s_{\mu\nu}$	Elastic compliance	$c_{\mu\nu}$	Elastic stiffness	$\sigma\sigma$
$Q_{\mu\nu}^\dagger$	Electrostriction	$\pi_{\mu\nu}^\dagger$	Piezo-optics	

† For contracted notation, see Section 1.1.4.10.5.