

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

provided by the *conversion equations* that express Cartesian tensor components as linear combinations of principal and secondary covariant components (for more details on tensorial covariants and conversion equations see Appendix E of the manual for *GI★KoBo-1* and Kopský, 2001).

We illustrate the situation on a transition with symmetry descent $4_2 2_x 2_{xy} \Downarrow 2_x 2_y 2_z$. In Table 3.1.3.1, we find that the principal tensor parameter transforms according to irreducible representation B_1 with standard variable x_3 . The corresponding covariant $u_3 = u_1 - u_2$ can be found in Appendix E of the manual of *GI★KoBo-1* (or in Kopský, 2001), where one also finds an invariant containing u_1 and u_2 : $u_{1,1} = u_1 + u_2$. The corresponding conversion equations are: $u_1 = \frac{1}{2}(u_{1,1} + u_3)$, $u_2 = \frac{1}{2}(u_{1,1} - u_3)$. In the parent phase $u_3 = u_1^{(p)} - u_2^{(p)} = 0$, hence $u_1^{(p)} = u_2^{(p)} = \frac{1}{2}u_{1,1}$, whereas in the ferroic phase $u_1^{(f)} = \frac{1}{2}(u_{1,1} + u_3) = u_1^{(p)} + \frac{1}{2}u_{1,1} = u_1^{(p)} + \delta u_1$, $u_2^{(f)} = u_2^{(p)} - \frac{1}{2}u_{1,1} = u_2^{(p)} - \delta u_2 = u_1^{(p)} - \delta u_1$. The symmetry-breaking increments $\delta u_1 = -\delta u_2$ describe thus the changes of the Cartesian components that correspond to the nonzero principal tensor component $u_1 - u_2$.

An analogous situation occurs frequently in trigonal and hexagonal parent groups, where $u_1 - u_2$ (or $g_1 - g_2$) transforms like the first or second component of the principal tensor parameter. In these cases, the corresponding symmetry-breaking increments of Cartesian components are again related: $\delta u_1 = -\delta u_2$ (or $\delta g_1 = -\delta g_2$).

We note that relations like $A_{11} = -A_{12} = -A_{26}$ do not imply that these components transform as the standard variable. Though these components are proportional to the principal tensor parameter in the first domain state, they cannot be transformed to corresponding components in other domain states as easily as covariant tensor components of the principal tensor parameter.

In general, it is useful to consider a tensor parameter as a vector in the carrier space of the respective representation. Then the Cartesian components are projections of this vector on the Cartesian basis of the tensor space.

The presentation of the principal tensor parameters in the column *Principal tensor parameters* of this table is a compromise: whenever conversion equations lead to simple relations between morphic Cartesian components and/or symmetry-breaking increments, we present these relations, in some cases together with corresponding covariants. In the more complicated cases, only the covariants are given. The corresponding conversion equations and labelling of covariants are given at the beginning of that part of the table which covers hexagonal and cubic parent groups G . In the main tables of the software *GI★KoBo-1*, the principal tensor parameters and the secondary tensor parameters up to rank 4 are given consistently in covariant form. Labelling of covariant components and conversion equations are given in Appendix E of the manual.

The principal tensor parameters presented in Table 3.1.3.1 represent a particular choice of property tensors for standard variables given in the second column. To save space, property tensors are selected in the following way: polarization \mathbf{P} and strain u are always listed; if none of their components transform according to $D^{(n)}$, then components of one axial and one polar tensor (if available) appearing in Table 3.1.3.3 are given. Principal parameters of two different property tensors are separated by a semicolon. If two different components of the same property tensor transform in the same way, they are separated by a comma.

As tensor indices we use integers 1, 2, 3 instead of vector components x, y, z and contracted indices 1, 2, 3, 4, 5, 6 in matrix notation for pairs $xx, yy, zz, yz \approx zy, zx \approx xz, xy \approx yx$, respectively

Important note: To make Table 3.1.3.1 compatible with the software *GI★KoBo-1* and with Kopský (2001), coefficients of property tensors in matrix notation with contracted indices 4, 5, 6 do not contain the numerical factors 2 and 4 which are usually

Table 3.1.3.3. *Important property tensors*

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

Tensor components	Property	Tensor components	Property
ε	enantiomorphism		chirality
P_i	polarization	P_i	pyroelectricity
u_μ	strain	ε_{ij}	dielectric permittivity
g_μ	optical activity		
$d_{i\mu}$	piezoelectricity	$r_{i\mu}$	electro-optics
$A_{i\mu}$	electrogyration		
$\pi_{\mu\nu}$	piezo-optics	$Q_{\mu\nu}$	electrostriction

introduced to preserve a compact form (without these factors) of linear constitutive relations [see Chapter 1.1, Nye (1985) and especially Appendices E and F of Sirotnin & Shaskolskaya (1982)]. This explains the differences in matrix coefficients appearing in Table 3.1.3.1 and those presented in Chapter 1.1 or in Nye (1985) and in Sirotnin & Shaskolskaya (1982). Thus *e.g.* for the symmetry descent $6_z 2_x 2_y \Downarrow 3_z 2_x$, we find in Table 3.1.3.1 the principal tensor parameters $d_{11} = -d_{12} = -d_{26}$, whereas according to Chapter 1.1 or *e.g.* to Nye (1985) or Sirotnin & Shaskolskaya (1982) these coefficients for $F_1 = 3_z 2_x$ are related by equations $d_{11} = -d_{12} = -2d_{26}$.

Property tensors and symbols of their components that can be found in Table 3.1.3.1 are given in the left-hand half of Table 3.1.3.3. The right-hand half presents other tensors that transform in the same way as those on the left and form, therefore, covariant tensor components of the same form as those given in the column *Principal tensor parameters*. Principal and secondary tensor parameters for all property tensors that appear in Table 3.1.3.3 are available in the software *GI★KoBo-1*.

n_f : number of ferroic single domain states that differ in the primary order parameter η and in the principal tensor parameters.

n_a : number of ferroelastic single domain states. If $n_a = n_f$, $n_a < n_f$ or $n_a = 1$, the ferroic phase is, respectively, a full, partial or non-ferroelastic one.

n_e : number of ferroelectric single domain states. If $n_e = n_f$, $n_e < n_f$ or $n_e = 0, 1$, the ferroic phase is, respectively, a full, partial or non-ferroelectric one ($n = 0$ or $n = 1$ correspond to a non-polar or to a polar parent phase, respectively) (see Section 3.4.2).

3.1.3.4. *Examples*

Example 3.1.3.4.1. Phase transition in triglycine sulfate (TGS). Assume that the space groups of both parent (high-symmetry) and ferroic (low-symmetry) phases are known: $\mathcal{G} = P2_1/c (C_{2h}^5)$, $\mathcal{F}_1 = P2_1 (C_2^2)$. The same number of formula units in the primitive unit cell in both phases suggests that the transition is an equitranslational one. This conclusion can be checked in the lattice of equitranslational subgroups of the software *GI★KoBo-1*. There we find for the low-symmetry space group the symbol $P112_1(\mathbf{b}/4)$, where the vector in parentheses expresses the shift of the origin with respect to the conventional origin given in *IT A* (2005).

In Table 3.1.3.1, one finds that the corresponding point-group-symmetry descent $2_z/m_z \Downarrow 2_z$ is associated with irreducible representation $\Gamma_\eta = A_u$. The corresponding principal tensor parameters of lowest rank are the pseudoscalar ε (enantiomorphism or chirality) and the vector of spontaneous polarization with one nonzero morphic component P_3 – the transition is a proper ferroelectric one. The non-ferroelastic ($n_a = 1$) full ferroelectric phase has two ferroelectric domain states ($n_f = n_e = 2$). Other principal tensor parameters (morphic tensor components that transform according to Γ_η) are available in the software *GI★KoBo-1*: $g_1, g_2, g_3, g_6; d_{31}, d_{32}, d_{33}, d_{36}, d_{14}, d_{15}, d_{24}, d_{25}$. Property tensors with these components are listed in Table 3.1.3.3. As shown in Section 3.4.2, all these components