

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

GI★KoBo-1 and in Kopský (2001). The corresponding Cartesian tensor components are available in Section 1.1.4 and in standard textbooks (e.g. Nye, 1985; Sirotnin & Shaskolskaya, 1982).

(2) If

$$I_G(\tau_a^{(\omega(1))}) = F_1, \quad (3.4.2.39)$$

then any of $m = n_\tau/d_\alpha$ tensorial covariants $\tau_a^{(\omega)}$, $a = 1, 2, \dots, m$, is a possible principal tensor parameter $\varphi^{(1)}$ of the transition $G \supset F_1$. Any two of $n_f = |G| : |F_1|$ principal domain states differ in some, or all, components of these covariants. The principal tensor parameter φ plays a similar symmetric (but generally not thermodynamic) role as the order parameter η does in the Landau theory. Only for equitranslational phase transitions is one of the principal tensor parameters (that with the temperature-dependent coefficient) identical with the primary order parameter of the Landau theory (see Section 3.1.3).

(3) If

$$I_G(\tau_a^{(\omega(1))}) = L_1, \quad F_1 \subset L_1 \subset G, \quad (3.4.2.40)$$

then $\tau_a^{(\omega(1))}$ represents the secondary tensor parameter λ (see Section 3.1.3.2). There exist $n_\lambda = |G| : |L_1|$ secondary domain states $\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_{n_\lambda}$ that differ in λ . Unlike in the two preceding cases (1) and (2), several intermediate groups L_1, M_2, \dots (with secondary tensor parameters λ, μ, \dots) that fulfil condition (3.4.2.40) can exist.

Now we shall indicate how one can find particular property tensors that fulfil conditions (3.4.2.39) or (3.4.2.40). The solution of this group-theoretical task consists of three steps:

(i) For a given point-group symmetry descent $G \supset F_1$, or $G \supset L_1$, one finds the representation Γ_η that specifies the transformation properties of the principal, or secondary, tensor parameter, which plays the role of the order parameters in a continuum description. This task is called an inverse Landau problem (see Section 3.1.3 for more details). The solution of this problem is available in Tables 3.4.2.7 and 3.1.3.1, in the software *GI★KoBo-1* and in Kopský (2001), where the letters *A, B* signify one-dimensional irreducible representations, and letters *E* and *T* two- and three-dimensional ones. The dimensionality d_η , or d_λ , of the representation Γ_η , or Γ_λ , specifies the maximal number of independent components of the principal, or secondary, tensor parameter φ , or λ , respectively. ‘Reducible’ indicates that Γ_η is a reducible representation.

(ii) In Table 3.1.3.1 one finds in the second column, for a given G and Γ_η , or Γ_λ (first column), the standard variables designating in a standardized way the covariant tensor components of the principal, or secondary, tensor parameters (for more details see Section 3.1.3.1 and the manual of the software *GI★KoBo-1*). For two- and three-dimensional irreducible representations, this column contains relations that restrict the values of the components and thus reduce the number of independent components.

(iii) The association of covariant tensor components of property tensors with standard variables is tabulated for all irreducible representations in an abridged version in Table 3.1.3.1, in the

column headed *Principal tensor parameters*, and in full in the main table of the software *GI★KoBo-1* and of Kopský (2001).

Phase transitions associated with reducible representations are treated in detail only in the software *GI★KoBo-1* and in Kopský (2001). Fortunately, these phase transitions occur rarely in nature.

A rich variety of observed structural phase transitions can be found in Tomaszewski (1992). This database lists 3446 phase transitions in 2242 crystalline materials.

Example 3.4.2.4. *Morphic tensor components associated with $4_z/m_z m_x m_{xy} \supset 2_x m_y m_z$ symmetry descent*

(1) *Principal tensor parameters $\varphi^{(1)}$* . The representation Γ_η that specifies the transformation properties of the principal tensor parameter $\varphi^{(1)}$ (and for equitranslational phase transitions also the primary order parameter $\eta^{(1)}$) can be found in the first column of Table 3.1.3.1 for $G = 4_z/m_z m_x m_{xy}$ and $F_1 = 2_x m_y m_z$; the *R*-irreducible representation (*R*-irep) $\Gamma_\eta = E_u$. Therefore, the principal tensor parameter $\varphi^{(1)}$ (or the primary order parameter $\eta^{(1)}$) has two components $(\varphi_1^{(1)}, \varphi_2^{(1)})$ [or $(\eta_1^{(1)}, \eta_2^{(1)})$]. The standard variables are in the second column: $(x_1^-, 0)$. This means that only the first component $\varphi_1^{(1)}$ (or $\eta_1^{(1)}$) is nonzero. In the column *Principal tensor parameters*, one finds that $\varphi_1^{(1)} = P_1$ (or $\eta_1^{(1)} = P_1$), i.e. one principal tensor parameter is spontaneous polarization and the spontaneous polarization in the first domain state \mathbf{S}_1 is $P_{(s)} = (P, 00)$. Other principal tensor parameters can be found in the software *GI★KoBo-1* or in Kopský (2001), p. 185: $(g_4, 0)$, $(d_{11}, 0)$, $(d_{12}, 0)$, $(d_{13}, 0)$, $(d_{26}, 0)$, $(d_{35}, 0)$ (the physical meaning of the components is explained in Table 3.4.3.5).

(2) *Secondary tensor parameters $\lambda^{(1)}, \mu^{(1)}, \dots$*

In the group lattice (group–subgroup chains) in Fig. 3.1.3.1, one finds that the only intermediate group between $4_z/m_z m_x m_{xy}$ and $2_x m_y m_z$ is $L_1 = m_x m_y m_z$. In the same table of the software *GI★KoBo-1* or in Kopský (2001), one finds $\Gamma_\lambda = B_{1g}$ and the following one-dimensional secondary tensor parameters: $u_1 - u_2$; $A_{14} + A_{25}$, A_{36} ; $s_{11} - s_{22}$, $s_{13} - s_{23}$, $s_{44} - s_{55}$; $Q_{11} - Q_{22}$, $Q_{12} - Q_{21}$, $Q_{13} - Q_{23}$, $Q_{31} - Q_{32}$, $Q_{44} - Q_{55}$.

The use of covariant tensor components has two practical advantages:

Firstly, the change of tensor components at a ferroic phase transition is completely described by the appearance of new nonzero covariant tensor components. If needed, Cartesian tensor components corresponding to covariant components can be calculated by means of conversion equations, which express Cartesian tensor components as linear combinations of covariant tensor components [for details on tensor covariants and conversion equations see the manual and Appendix E of the software *GI★KoBo-1* and Kopský (2001)].

Secondly, calculation of property tensors in various domain states is substantially simplified: transformations of Cartesian tensor components, which are rather involved for higher-rank tensors, are replaced by a simpler transformation of covariant tensor components by matrices $D^{(n)}$ of the matrix representation of Γ_η , or of Γ_λ [see again the software *GI★KoBo-1* and Kopský

Table 3.4.2.4. *Morphic properties, tensor parameters, order parameters and domain states*

T, U, S, V: property tensors; TOP: designation of tensor or order parameter; Γ : representation of G expressing the transformation properties of TOP. The terms ‘full’ and ‘partial’ were introduced by Aizu (1970a).

Morphic property	TOP	Γ	Stabilizer of TOP	Domain states
Spontaneous components of tensor T	φ	Γ_φ	F_1	Principal (full) in tensor T
Spontaneous components of tensor U	ψ	Γ_ψ	F_1	Principal (full) in tensor U
Spontaneous components of tensor S	σ	Γ_σ	F_1	Principal (full) in tensor S
Spontaneous components of tensor V	λ	Γ_λ	$L_1, F_1 \subset L_1 \subset G$	Degenerate (partial) in tensor V
Primary order parameter	η	Γ_η	\mathcal{F}_1	Basic (microscopic)
Pseudoproper order parameter	ζ	Γ_η	\mathcal{F}_1	Basic (microscopic)
Secondary (improper) order parameter	ξ	Γ_ξ	$\mathcal{L}_1, \mathcal{F}_1 \subset \mathcal{L}_1 \subset \mathcal{G}$	Secondary (improper) microscopic