

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

The solution of the inverse Landau problem – *i.e.* the identification of the representation Γ_η relevant to symmetry descent $G \Downarrow F$ – enables one to determine the corresponding normal mode (so-called soft mode) of the transition (see *e.g.* Rousseau *et al.*, 1981). We note that this step requires additional knowledge of the crystal structure, whereas other conclusions of the analysis hold for *any* crystal structure with a given symmetry descent $G \Downarrow F$. Normal-mode determination reveals the dynamic microscopic nature of the instability of the crystal lattice which leads to the phase transition (for more details and examples, see Section 3.1.5).

The representation Γ_η further determines the principal tensor parameters associated with the primary order parameter η . If one of them is a vector (polarization) the soft mode is infrared-active in the parent phase; if it is a symmetric second-rank tensor (spontaneous strain), the soft mode is Raman active in this phase. Furthermore, the *R*-irep Γ_η determines the polynomial in components of η in the Landau free energy (basic invariant polynomials, called *integrity bases*, are available in the software *GI★KoBo-1* and in Kopský, 2001) and allows one to decide whether the necessary conditions of continuity of the transition (so-called Landau and Lifshitz conditions) are fulfilled.

(2) *Direct Landau problem of equitranslational phase transitions:* For a given space group \mathcal{G} of the parent phase and the *R*-irep Γ_η (specifying the transformation properties of the primary order parameter η), find the corresponding equitranslational space group \mathcal{F} of the ferroic phase. To solve this task, one first finds in Table 3.1.3.1 the point group F that corresponds to point group G of space group \mathcal{G} and to the given *R*-irep Γ_η . The point-group symmetry descent $G \Downarrow F$ thus obtained specifies uniquely the equitranslational subgroup \mathcal{F} of \mathcal{G} that can be found in the lattices of equitranslational subgroups of space groups available in the software *GI★KoBo-1* (see Section 3.1.6).

(3) *Secondary tensor parameters of an equitranslational phase transition $\mathcal{G} \Downarrow \mathcal{F}$:* These parameters are specified by the representation Γ_λ of G associated with a symmetry descent $\Gamma \Downarrow L$, where L is an intermediate group [see equation (3.1.3.1)]. In other words, the secondary tensor parameters of the transition $G \Downarrow F$ are identical with principal tensor parameters of the transition $G \Downarrow L$. To each intermediate group L there corresponds a set of secondary tensor parameters. All intermediate subgroups of a symmetry descent $G \Downarrow F$ can be deduced from lattices of subgroups in Figs. 3.1.3.1 and 3.1.3.2.

The representation Γ_λ specifies transformation properties of the secondary tensor parameter λ and thus determines *e.g.* its

infrared and Raman activity in the parent phase and enables one to make a mode analysis. Representation Γ_λ together with Γ_η determine the coupling between secondary and primary tensor parameters. The explicit form of these faint interactions (Aizu, 1973; Kopský, 1979*d*) can be found in the software *GI★KoBo-1* and in Kopský (2001).

(4) *Changes of property tensors at a ferroic phase transition.* These changes are described by tensor parameters that depend only on the point-group-symmetry descent $G \Downarrow F$. This means that *the same principal tensor parameters and secondary tensor parameters appear in all equitranslational and in all non-equitranslational transitions with the same $G \Downarrow F$.* The only difference is that in non-equitranslational ferroic phase transitions a principal tensor parameter corresponds to a secondary ferroic order parameter. It still plays a leading role in tensor distinction of domains, since it exhibits different values in any two ferroic domain states (see Section 3.4.2.3). Changes of property tensors at ferroic phase transitions are treated in detail in the software *GI★KoBo-1* and in Kopský (2001).

We note that Table 3.1.3.1 covers only those point-group symmetry descents $G \Downarrow F$ that are ‘driven’ by *R*-ireps of G . All possible point-group symmetry descents $G \Downarrow F$ are listed in Table 3.4.2.7. Principal and secondary tensor parameters of symmetry descents associated with reducible representations are combinations of tensor parameters appearing in Table 3.1.3.1 (for a detailed explanation, see the manual of the software *GI★KoBo-1* and Kopský, 2000). Necessary data for treating these cases are available in the software *GI★KoBo-1* and Kopský (2001).

3.1.3.3.1. Explanation of Table 3.1.3.1

Parent symmetry G : the short international (Hermann–Mauguin) and the Schoenflies symbol of the point group G of the parent phase are given. Subscripts specify the orientation of symmetry elements (generators) in the Cartesian crystallophysical coordinate system of the group G (see Figs. 3.4.2.3 and 3.4.2.4, and Tables 3.4.2.5 and 3.4.2.6).

R-irep Γ_η : physically irreducible representation Γ_η of the group G in the spectroscopic notation. This representation defines transformation properties of the primary order parameter η and of the principal tensor parameters. Each complex irreducible representation is combined with its complex conjugate and thus a real physically irreducible representation *R*-irep is formed. Matrices $D^{(\alpha)}$ of *R*-ireps are given explicitly in the the software *GI★KoBo-1*.

Table 3.1.3.2. Symmetry descents $G \Downarrow F_1$ associated with two irreducible representations

G	Γ_η	F_1	Proper or improper		Domain states			Full or partial	
			Ferroelectric	Ferroelastic	n_f	n_e	n_a	Ferroelectric	Ferroelastic
432	T_1	2_{xy}	proper	improper	12	12	12	full	full
	T_2		improper	proper					
	T_1	1	improper	improper	24	24	24	full	full
	T_2		proper	proper					
$\bar{4}3m$	T_1	m_{xy}	improper	improper	12	12	12	full	full
	T_2		proper	proper					
	T_1	1	improper	improper	24	24	24	full	full
	T_2		proper	proper					
$m\bar{3}m$	T_{1g}	$2_{xy}/m_{xy}$	non	improper	12	0	12	non	full
	T_{2g}		non	proper					
	T_{1g}	$\bar{1}$	non	improper	24	0	24	non	full
	T_{2g}		non	proper					
	T_{1u}	$m_{xy}2_{xy}m_z$	proper	improper	12	12	6	full	partial
	T_{2u}		improper	improper					
	T_{1u}	m_z	proper	improper	24	24	12	full	partial
	T_{2u}		improper	improper					
	T_{1u}	1	proper	improper	48	48	24	full	partial
	T_{2u}		improper	improper					