

3. PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

$$\begin{aligned} N &= [G : \mathcal{F}] = [G : F][\mathbf{T} : \mathbf{U}] \\ &= (|G| : |F|)(v_{\mathcal{F}} : v_G) = (|G| : |F|)(Z_{\mathcal{F}} : Z_G) \\ &= (|G| : |F|)\det(m_{ij}) = nd_i. \end{aligned} \quad (3.2.3.91)$$

Each suborbit, represented by a row in the array (3.2.3.84), contains all basic (microscopic) domain states that are related by pure translations. These domain states exhibit the same tensor properties, *i.e.* they belong to the same ferroic domain state.

Example [sT] 3.2.3.33. Let us consider a phase transition with a symmetry descent $G \supset F_1$ with an orbit $G\mathbf{S}_{11}$ of domain states. Let L_1 be an intermediate group, $F_1 \subset L_1 \subset G$, and $\lambda^{(1)}$ the principal order parameter associated with the symmetry descent $G \supset L_1$ [cf. (3.2.3.58)], $I_G(\lambda^{(1)}) = L_1$. Since L_1 is an intermediate group, the quantity $\lambda^{(1)}$ represents a secondary order parameter of the symmetry descent $G \supset F_1$. The G orbit of $\lambda^{(1)}$ is

$$G\lambda^{(1)} = \{\lambda^{(1)}, \lambda^{(2)}, \dots, \lambda^{(m)}\}, \quad m = [G : L_1]. \quad (3.2.3.92)$$

As in Example [oT] 3.2.3.28, there is a bijection between left cosets of the decomposition of G into left cosets of L_1 [see (3.2.3.80)] and the G orbit of secondary order parameters (3.2.3.92). One can, therefore, associate with the suborbit $L_j\mathbf{S}_{j1}$ the value $\lambda^{(j)}$ of the secondary order parameter λ ,

$$L_j\mathbf{S}_{j1} \leftrightarrow \lambda^{(j)}, \quad j = 1, 2, \dots, m. \quad (3.2.3.93)$$

A suborbit $L_j\mathbf{S}_{j1}$ is thus comprised of objects of the orbit $G\mathbf{S}_{11}$ with the same value of the secondary order parameter $\lambda^{(j)}$.

Example [oS] 3.2.3.34. Let us choose for the intermediate group L_1 the normalizer $N_G(F_1)$. Then the suborbits equal

$$\begin{aligned} N_G(F_j)\mathbf{S}_{j1} &= \{h_j\mathbf{S}_{11}, h_j p_2\mathbf{S}_{11}, \dots, h_j p_d\mathbf{S}_{11}\}, \\ j &= 1, 2, \dots, m = [G : N_G(F_1)], \end{aligned} \quad (3.2.3.94)$$

where $p_1 = e, p_2, \dots, p_d$ are representatives of left cosets $p_k F_1$ in the decomposition of $N_G(F_1)$,

$$N_G(F_1) = p_1 F_1 \cup p_2 F_1 \cup \dots \cup p_d F_1, \quad d = [N_G(F_1) : F_1], \quad (3.2.3.95)$$

and h_j are representatives of the decomposition (3.2.3.77). The suborbit $F_j\mathbf{S}_{j1}$ consists of all objects with the same stabilizer F_j ,

$$\begin{aligned} I_G(\mathbf{S}_{j1}) &= I_G(\mathbf{S}_{j2}) = \dots = I_G(\mathbf{S}_{jd}) = F_j, \\ j &= 1, 2, \dots, m = [G : N_G(F_1)]. \end{aligned} \quad (3.2.3.96)$$

Propositions 3.2.3.23 and 3.2.3.30 are examples of structures that a group action induces from a group G on a G -set. Another important example is a permutation representation of the group G which associates operations of G with permutations of the objects of the orbit $G\mathbf{S}_i$ [see *e.g.* Kerber (1991, 1999); for application of the permutation representation in domain-structure analysis and domain engineering, see *e.g.* Fuksa & Janovec (1995, 2002)].

3.2.3.3.6. Orbits of ordered pairs and double cosets

An ordered pair $(\mathbf{S}_i, \mathbf{S}_k)$ is formed by two objects $\mathbf{S}_i, \mathbf{S}_k$ from the orbit $G\mathbf{S}_1$. Let \mathbf{P} denote the set of all ordered pairs that can be formed from the objects of the orbit $G\mathbf{S}_1$. The group action φ of group G on the set \mathbf{P} is defined by the following relation:

$$\begin{aligned} \varphi : g(\mathbf{S}_i, \mathbf{S}_k) &= (g\mathbf{S}_i, g\mathbf{S}_k) = (\mathbf{S}_r, \mathbf{S}_s), \\ g &\in G, \quad (\mathbf{S}_i, \mathbf{S}_k), (\mathbf{S}_r, \mathbf{S}_s) \in \mathbf{P}. \end{aligned} \quad (3.2.3.97)$$

The requirements (3.2.3.47) to (3.2.3.49) are fulfilled, mapping (3.2.3.97) defines an action of group G on the set \mathbf{P} .

The group action (3.2.3.97) introduces the G -equivalence of ordered pairs: Two ordered pairs $(\mathbf{S}_i, \mathbf{S}_k)$ and $(\mathbf{S}_r, \mathbf{S}_s)$ are crystallographically equivalent (with respect to the group G), $(\mathbf{S}_i, \mathbf{S}_k) \stackrel{G}{\sim} (\mathbf{S}_r, \mathbf{S}_s)$, if there exists an operation $g \in G$ that transforms $(\mathbf{S}_i, \mathbf{S}_k)$ into $(\mathbf{S}_r, \mathbf{S}_s)$,

$$g \in G \quad (g\mathbf{S}_i, g\mathbf{S}_k) = (\mathbf{S}_r, \mathbf{S}_s), \quad (\mathbf{S}_i, \mathbf{S}_k), (\mathbf{S}_r, \mathbf{S}_s) \in \mathbf{P}. \quad (3.2.3.98)$$

An orbit of ordered pairs $G(\mathbf{S}_i, \mathbf{S}_k)$ comprises all ordered pairs crystallographically equivalent with $(\mathbf{S}_i, \mathbf{S}_k)$. One can choose as a representative of the orbit $G(\mathbf{S}_i, \mathbf{S}_k)$ an ordered pair $(\mathbf{S}_1, \mathbf{S}_j)$ with the first member \mathbf{S}_1 since there is always an operation $g_{i1} \in G$ such that $g_{i1}\mathbf{S}_i = \mathbf{S}_1$. The orbit $F_1(\mathbf{S}_1, \mathbf{S}_j)$ assembles all ordered pairs with the first member \mathbf{S}_1 . This orbit can be expressed as

$$\begin{aligned} F_1(\mathbf{S}_1, \mathbf{S}_j) &= (F_1\mathbf{S}_1, F_1\mathbf{S}_j) = (\mathbf{S}_1, F_1(g_j\mathbf{S}_1)) \\ &= (\mathbf{S}_1, (F_1g_j)(F_1\mathbf{S}_1)) = (\mathbf{S}_1, (F_1g_jF_1)\mathbf{S}_1), \end{aligned} \quad (3.2.3.99)$$

where the identity $F_1\mathbf{S}_1 = \mathbf{S}_1$ [see relation (3.2.3.70)] has been used.

Thus the double coset $F_1g_jF_1$ contains all operations from G that produce all ordered pairs with the first member \mathbf{S}_1 that are G -equivalent with $(\mathbf{S}_1, \mathbf{S}_j = g_j\mathbf{S}_1)$. If one chooses $g_r \in G$ that is not contained in the double coset $F_1g_jF_1$, then the ordered pair $(\mathbf{S}_1, \mathbf{S}_r = g_r\mathbf{S}_1)$ must belong to another orbit $G(\mathbf{S}_1, \mathbf{S}_r) \neq G(\mathbf{S}_1, \mathbf{S}_j)$. Hence to distinct double cosets there correspond distinct classes of ordered pairs with the first member \mathbf{S}_1 , *i.e.* distinct orbits of ordered pairs. Since the group G can be decomposed into disjoint double cosets [see (3.2.3.36)], one gets

Proposition 3.2.3.35. Let G be a group and \mathbf{P} a set of all ordered pairs that can be formed from the objects of the orbit $G\mathbf{S}_1$. There is a one-to-one correspondence between the G orbits of ordered pairs of the set \mathbf{P} and the double cosets of the decomposition

$$G = F_1 \cup F_1g_2F_1 \cup \dots \cup F_1g_jF_1 \cup \dots \cup F_1g_qF_1, \quad j = 1, 2, \dots, q. \quad (3.2.3.100)$$

$$G(\mathbf{S}_1, \mathbf{S}_j) \leftrightarrow F_1g_jF_1 \text{ where } \mathbf{S}_j = g_j\mathbf{S}_1. \quad (3.2.3.101)$$

This bijection allows one to express the partition of the set \mathbf{P} of all ordered pairs into G orbits,

$$\mathbf{P} = G(\mathbf{S}_1, \mathbf{S}_1) \cup G(\mathbf{S}_1, g_2\mathbf{S}_1) \cup \dots \cup (\mathbf{S}_1, \mathbf{S}_j) \cup \dots \cup G(\mathbf{S}_1, g_q\mathbf{S}_1), \quad (3.2.3.102)$$

where $\{g_1 = e, g_2, \dots, g_j, \dots, g_q\}$ is the set of representatives of double cosets in the decomposition (3.2.3.100) (Janovec, 1972).

Proposition 3.2.3.35 applies directly to pairs of domain states (domain pairs) and allows one to find transposition laws that can appear in the low-symmetry phase (see Section 3.4.3).

For more details and other applications of group action see *e.g.* Kopský (1983), Lang (1965), Michel (1980), Opechowski (1986), Robinson (1982), and especially Kerber (1991, 1999).

References

Aizu, K. (1969). Possible species of "ferroelastic" crystals and of simultaneously ferroelectric and ferroelastic crystals. *J. Phys. Soc. Jpn*, **27**, 387–396.