

3.4. DOMAIN STRUCTURES

$$S_{jk} = h_j p_k S_{11}, \quad S_{11} = S_1, \quad j = 1, 2, \dots, n_\lambda, \quad k = 1, 2, \dots, d_\lambda, \quad (3.4.2.24)$$

where h_j and p_k are representatives of the decompositions (3.4.2.20) and (3.4.2.23), respectively.

The secondary order parameter λ can be identified with a principal order parameter of a phase transition with symmetry descent $G \subset L_1$ (see Section 3.4.2.3). The concept of secondary domain states enables one to define domain states that are characterized by a certain spontaneous property. We present the three most significant cases of such ferroic domain states.

3.4.2.2.1. Ferroelastic domain state

The distinction ferroelastic–non-ferroelastic is a basic division in domain structures. *Ferroelastic transitions* are ferroic transitions involving a spontaneous distortion of the crystal lattice that entails a change of shape of the crystallographic or conventional unit cell (Wadhawan, 2000). Such a transformation is accompanied by a change in the number of independent nonzero components of a symmetric second-rank tensor u that describes spontaneous strain.

In discussing ferroelastic and non-ferroelastic domain structures, the concepts of crystal family and holohedry of a point group are useful (IT A, 2005). Crystallographic point groups (and space groups as well) can be divided into seven crystal systems and six *crystal families* (see Table 3.4.2.2). A symmetry descent within a crystal family does not entail a qualitative change of the spontaneous strain – the number of independent nonzero tensor components of the strain tensor u remains unchanged.

We shall call the largest group of the crystal family to which the group M belongs the *family group of M* (symbol FamM). Then a simple criterion for a ferroic phase transition with symmetry descent $G \subset F$ to be a *non-ferroelastic phase transition* is

$$F \subset G, \quad \text{Fam}F = \text{Fam}G. \quad (3.4.2.25)$$

A necessary and sufficient condition for a *ferroelastic phase transition* is

$$F \subset G, \quad \text{Fam}F \neq \text{Fam}G. \quad (3.4.2.26)$$

A *ferroelastic domain state* R_i is defined as a state with a homogeneous spontaneous strain $u^{(i)}$. [We drop the suffix ‘s’ or ‘(s)’ if the serial number of the domain state is given as the superscript (i). The definition of spontaneous strain is given in Section 3.4.3.6.1.] Different ferroelastic domain states differ in spontaneous strain. The symmetry of a ferroelastic domain state R_i is specified by the stabilizer $I_G(u^{(i)})$ of the spontaneous strain $u^{(i)}$ of the principal domain state S_i [see (3.4.2.16)]. This stabilizer, which we shall denote by A_i , can be expressed as an intersection of the parent group G and the family group of F_i (see Table 3.4.2.2):

$$A_i \equiv I_G(u^{(i)}) = G \cap \text{Fam}F_i. \quad (3.4.2.27)$$

This equation indicates that the ferroelastic domain state R_i has a prominent single-domain orientation. Further on, the term ‘ferroelastic domain state’ will mean a ‘ferroelastic domain state in single-domain orientation’.

In our illustrative example,

$$\begin{aligned} A_1 &= I_{4_z/m_z m_x m_{xy}}(u_{11} - u_{22}) \\ &= \text{Fam}(2_x m_y m_z) \cap m 4_z / m_z m_x m_{xy} \\ &= m_x m_y m_z \cap 4_z / m_z m_x m_{xy} = m_x m_y m_z. \end{aligned}$$

The number n_a of ferroelastic domain states is given by

$$n_a = [G : A_1] = |G| : |A_1|. \quad (3.4.2.28)$$

In our example, $n_a = |4_z/m_z m_x m_{xy}| : |m_x m_y m_z| = 16 : 8 = 2$. In Table 3.4.2.7, last column, the number n_a of ferroelastic domain states is given for all possible ferroic phase transitions.

The number d_a of principal domain states compatible with one ferroelastic domain state (degeneracy of ferroelastic domain states) is given by

$$d_a = [A_1 : F_1] = |A_1| : |F_1|. \quad (3.4.2.29)$$

In our example, $d_a = |m_x m_y m_z| : |2_x m_y m_z| = 8 : 4 = 2$, i.e. two non-ferroelastic principal domain states are compatible with each of the two ferroelastic domain states (cf. Fig. 3.4.2.2).

The product of n_a and d_a is equal to the number n of all principal domain states [see equation (3.4.2.19)],

$$n_a d_a = [G : A_1][A_1 : F_1] = [G : F_1] = n. \quad (3.4.2.30)$$

The number d_a of principal domain states in one ferroelastic domain state can be calculated for all ferroic phase transitions from the ratio of numbers n and n_a that are given in Table 3.4.2.7.

According to Aizu (1969), we can recognize three possible cases (see also Table 3.4.2.3):

(i) *Full ferroelastics*: All principal domain states differ in spontaneous strain. In this case, $n_a = n$, i.e. $A_1 = F_1$, ferroelastic domain states are identical with principal domain states.

(ii) *Partial ferroelastics*: Some but not all principal domain states differ in spontaneous strain. A necessary and sufficient condition is $1 < n_a < n$, or, equivalently, $F_1 \subset A_1 \subset G$. In this case, ferroelastic domain states are degenerate secondary domain states with degeneracy $n > d_a = |A_1| : |F_1| > 1$. In this case, the phase transition $G \supset F_1$ can also be classified as an *improper ferroelastic* one (see Section 3.1.3.2).

(iii) *Non-ferroelastics*: All principal domain states have the same spontaneous strain. The criterion is $n_a = 1$, i.e. $A_1 = G$.

Example 3.4.2.1. Domain states in leucite. Leucite (KAlSi₂O₆) (see e.g. Hatch *et al.*, 1990) undergoes at about 938 K a ferroelastic phase transition from cubic symmetry $G = m\bar{3}m$ to tetragonal symmetry $L = 4/mmm$. This phase can appear in $|m\bar{3}m| : |4/mmm| = 3$ single-domain states, which we denote R_1, R_2, R_3 . The symmetry group of the first domain state R_1 is

Table 3.4.2.2. Crystal systems, holohedries, crystal families and number of spontaneous strain components

Point group M	Crystal system	Holohedry HolM	Spontaneous strain components		Crystal family	Family group FamM
			Independent	Nonzero		
23, $m\bar{3}$, 432, $\bar{4}3m$, $m\bar{3}m$	Cubic	$m\bar{3}m$	1	3	Cubic	$m\bar{3}m$
6, $\bar{6}$, 6/m, 622, 6mm, $\bar{6}2m$, 6/mmmm	Hexagonal	6/mmm	2	3	Hexagonal	6/mmm
3, $\bar{3}$, 32, 3m, $\bar{3}m$	Trigonal	$\bar{3}m$	2	3		
4, $\bar{4}$, 4/m, 422, 4mm, $\bar{4}2m$, 4/mmm	Tetragonal	4/mmm	2	3	Tetragonal	4/mmm
222, mm2, mmm	Orthorhombic	mmm	3	3	Orthorhombic	mmm
2, m, 2/m	Monoclinic	2/m	4	4	Monoclinic	2/m
1, $\bar{1}$	Triclinic	$\bar{1}$	6	6	Triclinic	$\bar{1}$