International Tables for Crystallography (2013). Vol. D, Figure 3.4.2.1, p. 487.

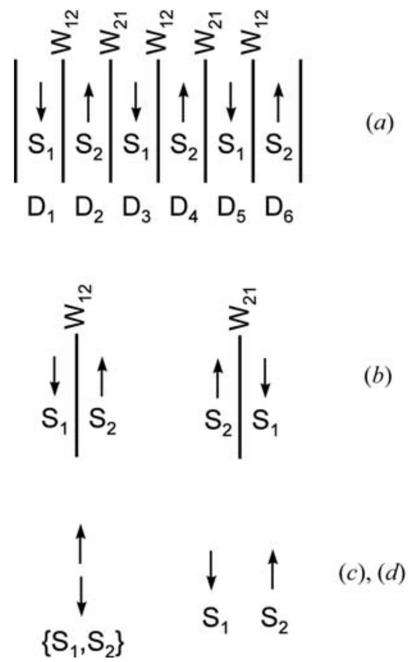

Fig. 3.4.2.1. Hierarchy in domain-structure analysis. (*a*) Domain structure consisting of domains $\mathbf{D}_1, \mathbf{D}_2, \ldots, \mathbf{D}_6$ and domain walls $\mathbf{W}_{12}$ and $\mathbf{W}_{21}$; (*b*) domain twin and reversed twin (with reversed order of domain states); (*c*) domain pair consisting of two domain states $\mathbf{S}_1$ and $\mathbf{S}_2$; (*d*) domain states $\mathbf{S}_1$ and $\mathbf{S}_2$.

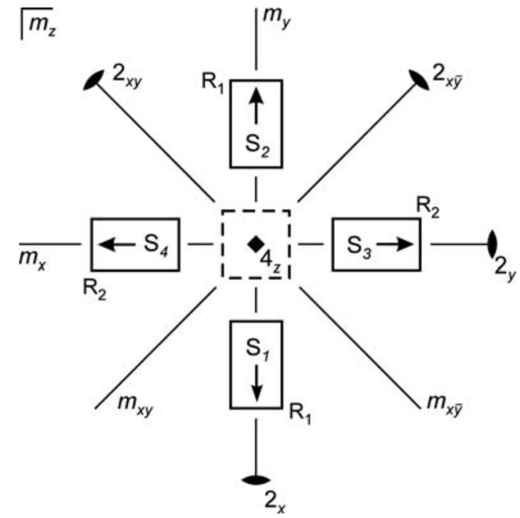

Fig. 3.4.2.2. Exploded view of single-domain states $\mathbf{S}_1$, $\mathbf{S}_2$, $\mathbf{S}_3$ and $\mathbf{S}_4$ (solid rectangles with arrows of spontaneous polarization) formed at a phase transition from a parent phase with symmetry $G = 4_z/m_zm_xm_{xy}$ to a ferroic phase with symmetry $F_1 = 2_xm_ym_z$. The parent phase is represented by a dashed square in the centre with the symmetry elements of the parent group $G = 4_z/m_zm_xm_{xy}$ shown.

homogeneous low-symmetry crystal structure. *Domain walls* can be associated with the boundaries of domain regions. The interior homogeneous bulk structure within a domain region will be called a *domain state*. Equivalent terms are *variant* or *structural variant* (Van Tendeloo & Amelinckx, 1974). We shall use different adjectives to specify domain states. In the microscopic description, domain states associated with the primary order parameter will be referred to as *primary* (*microscopic*, *basic*) *domain states*. Corresponding domain states in the macroscopic description will be called *principal domain states*, which correspond to Aizu's *orientation states*. (An exact definition of principal domain states is given below.)

Further useful division of domain states is possible (though not generally accepted): Domain states that are specified by a constant value of the spontaneous strain are called *ferroelastic domain states*; similarly, *ferroelectric domain states* exhibit constant spontaneous polarization *etc*. Domain states that differ in some tensor properties are called *ferroic* or *tensorial domain states etc*. If no specification is given, the statements will apply to any of these domain states.

A domain $\mathbf{D}_i$ is specified by a domain state $\mathbf{S}_j$ and by domain region Q_k: $\mathbf{D}_i = \mathbf{D}_i(\mathbf{S}_j, Q_k)$. Different domains may possess the same domain state but always differ in the domain region that specifies their shape and position in space.

The term 'domain' has also often been used for a domain state. Clear distinction of these two notions is essential in further considerations and is illustrated in Fig. 3.4.2.1. A ferroelectric domain structure (Fig. 3.4.2.1*a*) consists of six ferroelectric domains $\mathbf{D}_1, \mathbf{D}_2, \ldots, \mathbf{D}_6$ but contains only two domain states $\mathbf{S}_1, \mathbf{S}_2$ characterized by opposite directions of the spontaneous polarization depicted in Fig. 3.4.2.1(*d*). Neighbouring domains have different domain states but non-neighbouring domains may possess the same domain state. Thus domains with odd serial number have the domain state $\mathbf{S}_1$ (spontaneous polarization 'down'), whereas domains with even number have domain state $\mathbf{S}_2$ (spontaneous polarization 'up').

A great diversity of observed domain structures are connected mainly with various dimensions and shapes of domain regions, whose shapes depend sensitively on many factors (kinetics of the phase transition, local stresses, defects *etc*.). It is, therefore, usually very difficult to interpret in detail a particular observed domain pattern. Domain states of domains are, on the other hand, governed by simple laws, as we shall now demonstrate.

We shall consider a ferroic phase transition with a symmetry lowering from a parent (prototypic, high-symmetry) phase with symmetry described by a point group G to a ferroic phase with the point-group symmetry F_1, which is a subgroup of G. We shall denote this dissymmetrization by a group–subgroup symbol $G \supset F_1$ (or $G \Downarrow F_1$ in Section 3.1.3) and call it a *symmetry descent*, *dissymmetrization*, symmetry lowering or reduction.

As an illustrative example, we choose a phase transition with parent symmetry $G = 4_z/m_zm_xm_{xy}$ and ferroic symmetry $F_1 = 2_xm_ym_z$ (see Fig. 3.4.2.2). Strontium bismuth tantalate (SBT) crystals, for instance, exhibit a phase transition with this symmetry descent (Chen *et al.*, 2000). Symmetry elements in the symbols of G and F_1 are supplied with subscripts specifying the orientation of the symmetry elements with respect to the reference coordinate system. The necessity of this extended notation is exemplified by the fact that the group $G = 4_z/m_zm_xm_{xy}$ has six subgroups with the same 'non-oriented' symbol $mm2$: $m_xm_y2_z$, $2_xm_ym_z$, $m_x2_ym_z$, $m_{x\bar{y}}m_{xy}2_z$, $2_{x\bar{y}}m_{xy}m_z$, $m_{x\bar{y}}2_{xy}m_z$. Lower indices thus specify these subgroups unequivocally and the example illustrates an important rule of domain-structure analysis: *All symmetry operations, groups and tensor components must be related to a common reference coordinate system and their orientation in space must be clearly specified.*

The physical properties of crystals in the continuum description are expressed by property tensors. As explained in Section 1.1.4, the crystal symmetry reduces the number of independent components of these tensors. Consequently, for each property tensor the number of independent components in the low-symmetry ferroic phase is the same or higher than in the high-symmetry parent phase. Those tensor components or their linear combinations that are zero in the high-symmetry phase and nonzero in the low-symmetry phase are called *morphic tensor components* or *tensor parameters* and the quantities that appear only in the low-symmetry phase are called *spontaneous quantities* (see Section 3.1.3.2). The morphic tensor components and spontaneous quantities thus reveal the difference between the high- and low-symmetry phases. In our example, the symmetry $F_1 = 2_xm_ym_z$ allows a nonzero spontaneous polarization $\mathrm{P}_0^{(1)} = (P, 0, 0)$, which must be zero in the high-symmetry phase with $G = 4_z/m_zm_xm_{xy}$.

  references