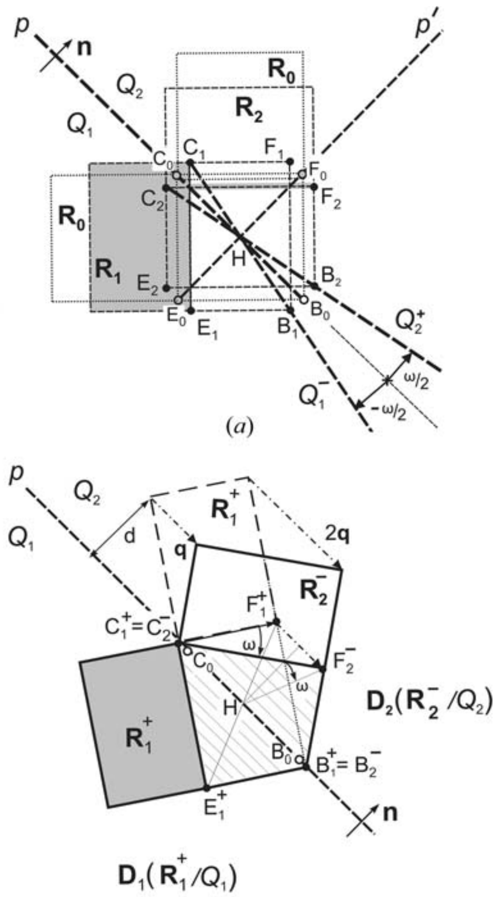
International Tables for Crystallography (2013). Vol. D, Figure 3.4.3.5, p. 517.



(*b*)

Fig. 3.4.3.5. Two ways of constructing a ferroelastic domain twin. (*a*) Formation of ferroelastic single-domain states $\mathbf{R}_1$, $\mathbf{R}_2$ from the parent phase state $\mathbf{R}_0$ and then rotating away these single-domain states through an angle $\pm\frac{1}{2}\omega$ about the domain-pair axis H so that disoriented ferroelastic domain states $\mathbf{R}_1^+$ and $\mathbf{R}_2^-$ meet along one of two perpendicular planes of equal deformation p or p'. (*b*) Formation of a ferroelastic twin from one ferroelastic domain state $\mathbf{R}_1^+$ by a simple shear deformation with a shear angle (obliquity) ω. For more details see the text.

$$\mathbf{u}_{(s)}^{(1)} = \mathbf{u}^{(1)} - \mathbf{u}^{(\mathrm{av})} = \begin{pmatrix} \frac{1}{2}(u_{11}-u_{22}) & 0 & 0 \\ 0 & -\frac{1}{2}(u_{11}-u_{22}) & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{3.4.3.49}$$

$$\mathbf{u}_{(s)}^{(2)} = \mathbf{u}^{(2)} - \mathbf{u}^{(\mathrm{av})} = \begin{pmatrix} -\frac{1}{2}(u_{11}-u_{22}) & 0 & 0 \\ 0 & \frac{1}{2}(u_{11}-u_{22}) & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{3.4.3.50}$$

Symmetry-breaking nonzero components of the relative spontaneous strain are identical, up to the factor $\frac{1}{2}$, with the secondary tensor parameters $\lambda_b^{(1)}$ and $\lambda_b^{(2)}$ of the transition $4_z/m_zm_xm_{xy} \supset 2_xm_ym_z$ with the stabilizer $I_{4_z/m_zm_xm_{xy}}(\mathbf{R}_1) = I_{4_z/m_zm_xm_{xy}}(\mathbf{R}_2) = m_xm_ym_z$. The non-symmetry-breaking component u_{33} does not appear in the relative spontaneous strain.

The form of relative spontaneous strains for all ferroelastic domain states of all full ferroelastic phases are listed in Aizu (1970*b*).

3.4.3.6.2. *Equally deformed planes of a ferroelastic domain pair*

We start with the example of a phase transition with the symmetry descent $G = 4_z/m_zm_xm_{xy} \supset 2_xm_ym_z$, which generates two ferroelastic single-domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ (see Fig. 3.4.2.2). An 'elementary cell' of the parent phase is represented in Fig. 3.4.3.5(*a*) by a square $B_0E_0C_0F_0$ and the corresponding domain state is denoted by $\mathbf{R}_0$.

In the ferroic phase, the square $B_0E_0C_0F_0$ can change either under spontaneous strain $\mathbf{u}^{(1)}$ into a spontaneously deformed rectangular cell $B_1E_1C_1F_1$ representing a domain state $\mathbf{R}_1$, or under a spontaneous strain $\mathbf{u}^{(2)}$ into rectangular $B_2E_2C_2F_2$ representing domain state $\mathbf{R}_2$. We shall use the letter $\mathbf{R}_0$ as a symbol of the parent phase and $\mathbf{R}_1$, $\mathbf{R}_2$ as symbols of two ferroelastic single-domain states.

Let us now choose in the parent phase a vector $\overrightarrow{HB_0}$. This vector changes into $\overrightarrow{HB_1}$ in ferroelastic domain state $\mathbf{R}_1$ and into $\overrightarrow{HB_2}$ in ferroelastic domain state $\mathbf{R}_1$. We see that the resulting vectors $\overrightarrow{HB_1}$ and $\overrightarrow{HB_2}$ have different direction but equal length: $|\overrightarrow{HB_1}| = |\overrightarrow{HB_2}|$. This consideration holds for any vector in the plane p, which can therefore be called an *equally deformed plane* (EDP). One can find that the perpendicular plane p' is also an equally deformed plane, but there is no other plane with this property.

The intersection of the two perpendicular equally deformed planes p and p' is a line called an *axis of the ferroelastic domain pair* $(\mathbf{R}_1, \mathbf{R}_2)$ (in Fig. 3.4.3.5 it is a line at H perpendicular to the paper). This axis is the only line in which any vector chosen in the parent phase exhibits equal deformation and has its direction unchanged in both single-domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ of a ferroelastic domain pair.

This consideration can be expressed analytically as follows (Fousek & Janovec, 1969; Sapriel, 1975). We choose in the parent phase a plane p and a unit vector $\mathbf{v}(x_1, x_2, x_3)$ in this plane. The changes of lengths of this vector in the two ferroelastic domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ are $u_{ik}^{(1)}x_ix_k$ and $u_{ik}^{(2)}x_ix_k$, respectively, where $u_{ik}^{(1)}$ and $u_{ik}^{(2)}$ are spontaneous strains in $\mathbf{R}_1$ and $\mathbf{R}_2$, respectively (see *e.g.* Nye, 1985). (We are using the Einstein summation convention: when a letter suffix occurs twice in the same term, summation with respect to that suffix is to be understood.) If these changes are equal, *i.e.* if

$$u_{ik}^{(1)}x_ix_k = u_{ik}^{(2)}x_ix_k, \tag{3.4.3.51}$$

for any vector $\mathbf{v}(x_1, x_2, x_3)$ in the plane p, then this plane will be an equally deformed plane. If we introduce a *differential spontaneous strain*

$$\Delta u_{ik} \equiv u_{ik}^{(2)} - u_{ik}^{(1)}, \quad i, k = 1, 2, 3, \tag{3.4.3.52}$$

the condition (3.4.3.51) can be rewritten as

$$\Delta u_{ik}x_ix_j = 0. \tag{3.4.3.53}$$

This equation describes a cone with the apex at the origin. The cone degenerates into two planes if the determinant of the differential spontaneous strain tensor equals zero,

$$\det\Delta u_{ik} = 0. \tag{3.4.3.54}$$

If this condition is satisfied, two solutions of (3.4.3.53) exist:

$$Ax_1 + Bx_2 + Cx_3 = 0, \quad A'x_1 + B'x_2 + C'x_3 = 0. \tag{3.4.3.55}$$

These are equations of two planes p and p' passing through the origin. Their normal vectors are $\mathbf{n} = [ABC]$ and $\mathbf{n}' = [A'B'C']$. It can be shown that from the equation

$$\Delta u_{11} + \Delta u_{22} + \Delta u_{33} = 0, \tag{3.4.3.56}$$

which holds for the trace of the matrix $\det\Delta u_{ik}$, it follows that these two planes are perpendicular:

$$AA' + BB' + CC' = 0. \tag{3.4.3.57}$$

The intersection of these equally deformed planes (3.4.3.53) is the *axis* $\mathbf{h}$ *of the ferroelastic domain pair* $(\mathbf{R}_1, \mathbf{R}_2)$.

references