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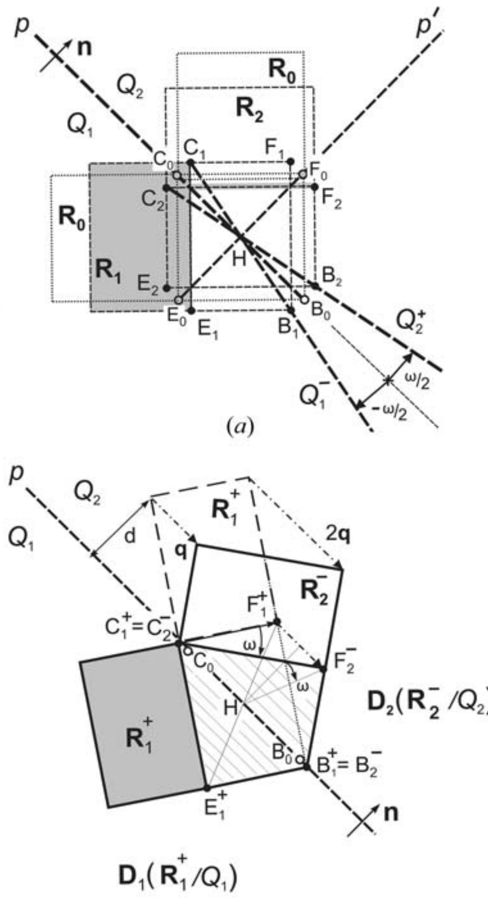

Fig. 3.4.3.5. Two ways of constructing a ferroelastic domain twin. (*a*) Formation of ferroelastic single-domain states $\mathbf{R}_1$, $\mathbf{R}_2$ from the parent phase state $\mathbf{R}_0$ and then rotating away these single-domain states through an angle $\pm\frac{1}{2}\omega$ about the domain-pair 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.

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

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

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

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

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*

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

the condition (3.4.3.51) can be rewritten as

$$\Delta u_{ik}x_ix_j = 0. \qquad (3.4.3.53)$$

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,

$$\det\Delta u_{ik} = 0. \qquad (3.4.3.54)$$

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

$$Ax_1 + Bx_2 + Cx_3 = 0, \quad A'x_1 + B'x_2 + C'x_3 = 0. \qquad (3.4.3.55)$$

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

$$\Delta u_{11} + \Delta u_{22} + \Delta u_{33} = 0, \qquad (3.4.3.56)$$

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

$$AA' + BB' + CC' = 0. \qquad (3.4.3.57)$$

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

Let us illustrate the application of these results to the domain pair $(\mathbf{R}_1, \mathbf{R}_2)$ depicted in Fig. 3.4.3.1(*b*) and discussed above. From equations (3.4.3.41) and (3.4.3.47), or (3.4.3.49) and (3.4.3.50) we find the only nonzero components of the difference strain tensor are

$$\Delta u_{11} = u_{22} - u_{11}, \quad \Delta u_{22} = u_{11} - u_{22}. \qquad (3.4.3.58)$$

Condition (3.4.3.54) is fulfilled and equation (3.4.3.53) is

$$\Delta u_{11} x_1^2 + \Delta u_{22} x_2^2 = (u_{22} - u_{11}) x_1^2 + (u_{11} - u_{22}) x_2^2 = 0. \qquad (3.4.3.59)$$

There are two solutions of this equation:

$$x_1 = x_2, \quad x_1 = -x_2. \qquad (3.4.3.60)$$

These two equally deformed planes p and p' have the normal vectors $\mathbf{n} = [\bar{1}10]$ and $\mathbf{n}' = [110]$. The axis $\mathbf{h}$ of this domain pair is directed along [001].

Equally deformed planes in our example have the same orientations as have the mirror planes $m_{\bar{x}y}$ and m_{xy} lost at the transition $4_z/m_z m_x m_{xy} \supset m_x m_y m_z$. From Fig. 3.4.3.5(*a*) it is clear why: reflection $m_{\bar{x}y}$, which is a transposing operation of the domain pair $(\mathbf{R}_1, \mathbf{R}_2)$, ensures that the vectors $\overrightarrow{HB_1}$ and $\overrightarrow{HB_2}$ arising from HB_0 have equal length. A similar conclusion holds for a 180° rotation and a plane perpendicular to the corresponding twofold axis. Thus we come to two useful rules:

Any reflection through a plane that is a transposing operation of a ferroelastic domain pair ensures the existence of two planes of equal deformation: one is parallel to the corresponding mirror plane and the other one is perpendicular to this mirror plane.

Any 180° rotation that is a transposing operation of a ferroelastic domain pair ensures the existence of two equally deformed planes: one is perpendicular to the corresponding twofold axis and the other one is parallel to this axis.

A reflection in a plane or a 180° rotation generates at least one equally deformed plane with a fixed prominent *crystallographic orientation* independent of the magnitude of the spontaneous strain; the other perpendicular equally deformed plane may have a *non-crystallographic orientation* which depends on the spontaneous strain and changes with temperature. If between switching operations there are two reflections with corresponding perpendicular mirror planes, or two 180° rotations with corresponding perpendicular twofold axes, or a reflection and a 180° rotation with a corresponding twofold axis parallel to the mirror, then both perpendicular equally deformed planes have fixed crystallographic orientations. If there are no switching operations of the second order, then both perpendicular equally deformed planes may have non-crystallographic orientations, or equally deformed planes may not exist at all.

Equally deformed planes in ferroelastic–ferroelectric phases have been tabulated by Fousek (1971). Sapriel (1975) lists equations (3.4.3.55) of equally deformed planes for all ferroelastic phases. Table 3.4.3.6 contains the orientation of equally deformed planes (with further information about the walls) for representative domain pairs of all orbits of ferroelastic domain pairs. Table 3.4.3.7 lists representative domain pairs of all ferroelastic orbits for which no compatible walls exist.

3.4.3.6.3. *Disoriented domain states, ferroelastic domain twins and their twin laws*

To examine another possible way of forming a ferroelastic domain twin, we return once again to Fig. 3.4.3.5(*a*) and split the space along the plane p into a half-space Q_1 on the negative side of the plane p (defined by a negative end of normal $\mathbf{n}$) and another half-space Q_2 on the positive side of p. In the parent phase, the whole space is filled with domain state $\mathbf{R}_0$ and we can, therefore, treat the crystal in region Q_1 as a domain $\mathbf{D}_1(\mathbf{R}_0, Q_1)$ and the crystal in region Q_2 as a domain $\mathbf{D}_2(\mathbf{R}_0, Q_2)$ (we remember that a domain is specified by its domain region, *e.g.* Q_1, and by a domain state, *e.g.* $\mathbf{R}_1$, in this region; see Section 3.4.2.1).

Now we cool the crystal down and exert the spontaneous strain $\mathbf{u}^{(1)}$ on domain $\mathbf{D}_1(\mathbf{R}_0, Q_1)$. The resulting domain $\mathbf{D}_1(\mathbf{R}_1, Q_1^-)$ contains domain state $\mathbf{R}_1$ in the domain region Q_1^- with the planar boundary along $(\overline{B_1C_1})$ (the overbar '−' signifies a rotation of the boundary in the positive sense). Similarly, domain $\mathbf{D}_2(\mathbf{R}_0, Q_2)$ changes after performing spontaneous strain $\mathbf{u}^{(2)}$ into domain $\mathbf{D}_2(\mathbf{R}_2, Q_2^+)$ with domain state $\mathbf{R}_2$ and the planar boundary along $(\overline{B_2C_2})$. This results in a disruption in the sector B_1AB_2 and in an overlap of $\mathbf{R}_1$ and $\mathbf{R}_2$ in the sector C_1AC_2.

The overlap can be removed and the continuity recovered by rotating the domain $\mathbf{D}_1(\mathbf{R}_1, Q_1^-)$ through angle $\omega/2$ and the domain $\mathbf{D}_2(\mathbf{R}_2, Q_2^+)$ through $-\omega/2$ about the domain-pair axis A (see Fig. 3.4.3.5*a* and *b*). This rotation changes the domain $\mathbf{D}_1(\mathbf{R}_1, Q_1^-)$ into domain $\mathbf{D}_1(\mathbf{R}_1^+, Q_1)$ and domain $\mathbf{D}_2(\mathbf{R}_2, Q_2^-)$ into domain $\mathbf{D}_1(\mathbf{R}_2^-, Q_2)$, where $\mathbf{R}_1^+$ and $\mathbf{R}_2^-$ are domain states rotated away from the single-domain state orientation through $\omega/2$ and $-\omega/2$, respectively. Domains $\mathbf{D}_1(\mathbf{R}_1, Q_1)$ and $\mathbf{D}_1(\mathbf{R}_2, Q_2)$ meet without additional strains or stresses along the plane p and form a *simple ferroelastic twin* with a *compatible domain wall* along p. This wall is stress-free and fulfils the conditions of mechanical compatibility.

Domain states $\mathbf{R}_1^+$ and $\mathbf{R}_2^-$ with new orientations are called *disoriented (misoriented) domain states* or *suborientational states* (Shuvalov *et al.*, 1985; Dudnik & Shuvalov, 1989) and the angles $\omega/2$ and $-\omega/2$ are the *disorientation angles* of $\mathbf{R}_1^+$ and $\mathbf{R}_2^-$, respectively.

We have described the formation of a ferroelastic domain twin by rotating single-domain states into new orientations in which a stress-free compatible contact of two ferroelastic domains is achieved. The advantage of this theoretical construct is that it provides a visual interpretation of disorientations and that it works with ferroelastic single-domain states which can be easily derived and transformed.

There is an alternative approach in which a domain state in one domain is produced from the domain state in the other domain by a shear deformation. The same procedure is used in mechanical twinning [for mechanical twinning, see Section 3.3.8.4 and *e.g.* Cahn (1954); Klassen-Neklyudova (1964); Christian (1975)].

We illustrate this approach again using our example. From Fig. 3.4.3.5(*b*) it follows that domain state $\mathbf{R}_2^-$ in the second domain can be obtained by performing a simple shear on the domain state $\mathbf{R}_1^+$ of the first domain. In this simple shear, a point is displaced in a direction parallel to the equally deformed plane p (in mechanical twinning called a *twin plane*) and to a plane perpendicular to the axis of the domain pair (*plane of shear*). The displacement $\mathbf{q}$ is proportional to the distance d of the point from the domain wall. The *amount of shear* is measured either by the absolute value of this displacement at a unit distance, $s = q/d$, or by an angle ω called a *shear angle* (sometimes 2ω is defined as the shear angle). There is no change of volume connected with a simple shear.

The angle ω is also called an *obliquity* of a twin (Cahn, 1954) and is used as a convenient measure of pseudosymmetry of the ferroelastic phase.

The high-resolution electron microscopy image in Fig. 3.4.3.6 reveals the relatively large shear angle (obliquity) ω of a ferroelastic twin in the monoclinic phase of tungsten trioxide (WO_3). The plane (101) corresponds to the plane p of a ferroelastic wall in Fig. 3.4.3.5(*b*). The planes $(\bar{1}01)$ are crystallographic planes in the lower and upper ferroelastic domains, which correspond in Fig. 3.4.3.5(*b*) to domain $\mathbf{D}_1(\mathbf{R}_1^+, Q_1)$ and domain $\mathbf{D}_2(\mathbf{R}_2^-, Q_2)$, respectively. The planes $(\bar{1}01)$ in these domains correspond to the diagonals of the elementary cells of $\mathbf{R}_1^+$ and $\mathbf{R}_2^-$ in Fig. 3.4.3.5(*b*) and are nearly perpendicular to the wall. The