

## 3. SYMMETRY ASPECTS OF PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

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

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

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

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

There are two solutions of this equation:

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

These two equally deformed planes  $p$  and  $p'$  have the normal vectors  $\mathbf{n} = [110]$  and  $\mathbf{n}' = [1\bar{1}0]$ . 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  $HB_1$  and  $HB_2$  arising from  $HB_0$  have equal length. A similar conclusion holds for a  $180^\circ$  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  $180^\circ$  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  $180^\circ$  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  $180^\circ$  rotations with corresponding perpendicular twofold axes, or a reflection and a  $180^\circ$  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  $(\bar{B}_1\bar{C}_1)$  (the overbar ‘ $\bar{\phantom{x}}$ ’ 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  $(\bar{B}_2\bar{C}_2)$ . 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. 3.4.3.5a 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  $\mathbf{D}_2(\mathbf{R}_2^-, Q_2)$ , 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  $\mathbf{D}_2(\mathbf{R}_2, Q_2)$  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  $\omega$  called a *shear angle* (sometimes  $2\omega$  is defined as the shear angle). There is no change of volume connected with a simple shear.

The angle  $\omega$  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)  $\omega$  of a ferroelastic twin in the monoclinic phase of tungsten trioxide ( $\text{WO}_3$ ). 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

### 3.4. DOMAIN STRUCTURES

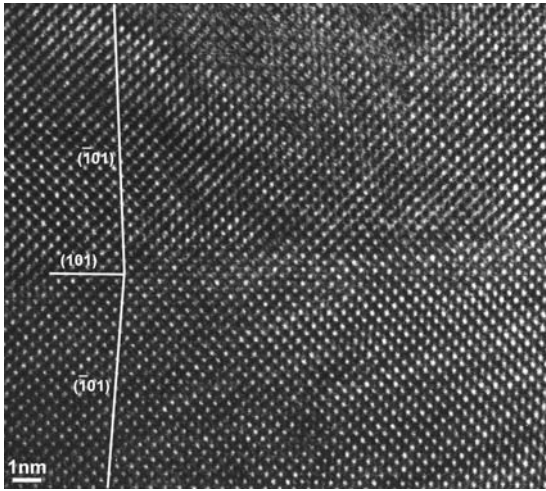


Fig. 3.4.3.6. High-resolution electron microscopy image of a ferroelastic twin in the orthorhombic phase of  $\text{WO}_3$ . Courtesy of H. Lemmens, EMAT, University of Antwerp.

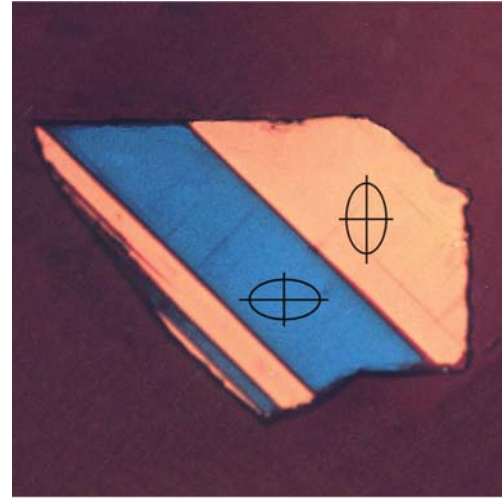
angle between these planes equals  $2\omega$ , where  $\omega$  is the shear angle (obliquity) of the ferroelastic twin.

Disorientations of domain states in a ferroelastic twin bring about a deviation of the optical indicatrix from a strictly perpendicular position. Owing to this effect, ferroelastic domains exhibit different colours in polarized light and can be easily visualized. This is illustrated for a domain structure of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  in Fig. 3.4.3.7. The symmetry descent  $G = 4_z/m_z m_x m_y \supset m_x m_y m_z = F_1 = F_2$  gives rise to two ferroelastic domain states  $\mathbf{R}_1$  and  $\mathbf{R}_2$ . The twinning group  $K_{12}$  of the non-trivial domain pair  $(\mathbf{R}_1, \mathbf{R}_2)$  is

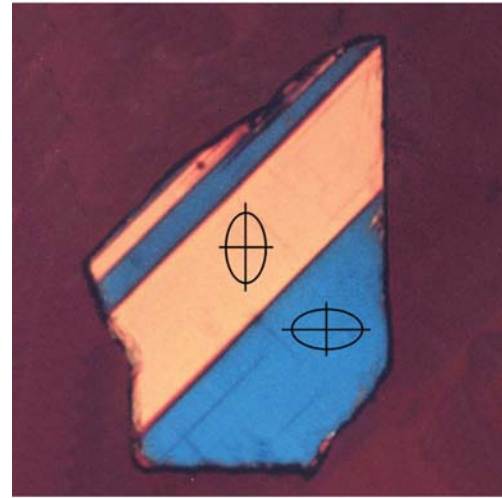
$$K_{12}[m_x m_y m_z] = J_{12}^* = m_x m_y m_z \cup 4_z^*[2_x m_y m_z] = 4_z^*/m_z m_x m_{xy}^*. \quad (3.4.3.61)$$

The colour of a domain state observed in a polarized-light microscope depends on the orientation of the index ellipsoid (indicatrix) with respect to a fixed polarizer and analyser. This index ellipsoid transforms in the same way as the tensor of spontaneous strain, *i.e.* it has different orientations in ferroelastic domain states. Therefore, different ferroelastic domain states exhibit different colours: in Fig. 3.4.3.7, the blue and pink areas (with different orientations of the ellipse representing the spontaneous strain in the plane of figure) correspond to two different ferroelastic domain states. A rotation of the crystal that does not change the orientation of ellipses (*e.g.* a  $180^\circ$  rotation about an axis parallel to the fourfold rotation axis) does not change the colours (ferroelastic domain states). If one neglects disorientations of ferroelastic domain states (see Section 3.4.3.6) – which are too small to be detected by polarized-light microscopy – then none of the operations of the group  $F_1 = F_2 = m_x m_y m_z$  change the single-domain ferroelastic domain states  $\mathbf{R}_1, \mathbf{R}_2$ , hence there is no change in the colours of domain regions of the crystal. On the other hand, all operations with a star symbol (operations lost at the transition) exchange domain states  $\mathbf{R}_1$  and  $\mathbf{R}_2$ , *i.e.* also exchange the two colours in the domain regions. The corresponding permutation is a transposition of two colours and this attribute is represented by a star attached to the symbol of the operation. This exchange of colours is nicely demonstrated in Fig. 3.4.3.7 where a  $-90^\circ$  rotation is accompanied by an exchange of the pink and blue colours in the domain regions (Schmid, 1991, 1993).

It can be shown (Shuvalov *et al.*, 1985; Dudnik & Shuvalov, 1989) that for small spontaneous strains the amount of shear  $s$  and the angle  $\omega$  can be calculated from the second invariant  $\Lambda_2$  of the differential tensor  $\Delta u_{ik}$ :



(a)



(b)

Fig. 3.4.3.7. Ferroelastic twins in a very thin  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  crystal observed in a polarized-light microscope. Courtesy of H. Schmid, Université de Geneve.

$$s = 2\sqrt{-\Lambda_2}, \quad (3.4.3.62)$$

$$\omega = \sqrt{-\Lambda_2}, \quad (3.4.3.63)$$

where

$$\Lambda_2 = \begin{vmatrix} \Delta u_{11} & \Delta u_{12} \\ \Delta u_{21} & \Delta u_{22} \end{vmatrix} + \begin{vmatrix} \Delta u_{22} & \Delta u_{23} \\ \Delta u_{32} & \Delta u_{33} \end{vmatrix} + \begin{vmatrix} \Delta u_{11} & \Delta u_{13} \\ \Delta u_{31} & \Delta u_{33} \end{vmatrix}. \quad (3.4.3.64)$$

In our example, where there are only two nonzero components of the differential spontaneous strain tensor [see equation (3.4.3.58)], the second invariant  $\Lambda_2 = -(\Delta u_{11} \Delta u_{22}) = -(u_{22} - u_{11})^2$  and the angle  $\omega$  is

$$\omega = \pm |u_{22} - u_{11}|. \quad (3.4.3.65)$$

In this case, the angle  $\omega$  can also be expressed as  $\omega = \pi/2 - 2 \arctan a/b$ , where  $a$  and  $b$  are lattice parameters of the orthorhombic phase (Schmid *et al.*, 1988).

The shear angle  $\omega$  ranges in ferroelastic crystals from minutes to degrees (see *e.g.* Schmid *et al.*, 1988; Dudnik & Shuvalov, 1989).

Each equally deformed plane gives rise to two compatible domain walls of the same orientation but with opposite sequence of domain states on each side of the plane. We shall use for a *simple domain twin* with a planar wall a symbol  $(\mathbf{R}_1^+ | \mathbf{n} | \mathbf{R}_2^-)$  in which  $\mathbf{n}$  denotes the normal to the wall. The bra-ket symbol  $( | )$  and  $( | )$  represents the half-space domain regions on the negative

### 3. SYMMETRY ASPECTS OF PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

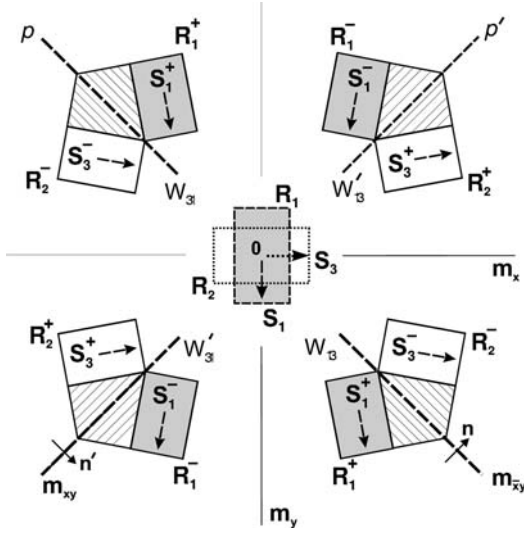


Fig. 3.4.3.8. Exploded view of four ferroelastic twins with disoriented ferroelastic domain states  $\mathbf{R}_1^+$ ,  $\mathbf{R}_2^-$  and  $\mathbf{R}_1^-$ ,  $\mathbf{R}_2^+$  formed from a single-domain pair ( $\mathbf{S}_1, \mathbf{S}_2$ ) (in the centre).

and positive sides of  $\mathbf{n}$ , respectively, for which we have used letters  $Q_1$  and  $Q_2$ , respectively. Then  $(\mathbf{R}_1^+ | \mathbf{R}_2^-)$  represent domains  $\mathbf{D}_1(\mathbf{R}_1^+, Q_1)$  and  $\mathbf{D}_2(\mathbf{R}_2^-, Q_2)$ , respectively. The symbol  $(\mathbf{R}_1^+ | \mathbf{R}_2^-)$  properly specifies a domain twin with a zero-thickness domain wall.

A domain wall can be considered as a domain twin with domain regions restricted to non-homogeneous parts near the plane  $p$ . For a domain wall in domain twin  $(\mathbf{R}_1^+ | \mathbf{R}_2^-)$  we shall use the symbol  $[\mathbf{R}_1^+ | \mathbf{R}_2^-]$ , which expresses the fact that a domain wall of zero thickness needs the same specification as the domain twin.

If we exchange domain states in the twin  $(\mathbf{R}_1^+ | \mathbf{n} | \mathbf{R}_2^-)$ , we get a *reversed twin (wall)* with the symbol  $(\mathbf{R}_2^- | \mathbf{n} | \mathbf{R}_1^+)$ . These two ferroelastic twins are depicted in the lower right and upper left parts of Fig. 3.4.3.8, where – for ferroelastic–non-ferroelectric twins – we neglect spontaneous polarization of ferroelastic domain states. The reversed twin  $\mathbf{R}_2^- | \mathbf{n} | \mathbf{R}_1^+$  has the opposite shear direction.

Twin and reversed twin can be, but may not be, crystallographically equivalent. Thus *e.g.* ferroelastic–non-ferroelectric twins  $(\mathbf{R}_1^+ | \mathbf{n} | \mathbf{R}_2^-)$  and  $(\mathbf{R}_2^- | \mathbf{n} | \mathbf{R}_1^+)$  in Fig. 3.4.3.8 are equivalent, *e.g. via*  $2_z$ , whereas ferroelastic–ferroelectric twins  $(\mathbf{S}_1^+ | \mathbf{n} | \mathbf{S}_3^-)$  and  $(\mathbf{S}_3^- | \mathbf{n} | \mathbf{S}_1^+)$  are not equivalent, since there is no operation in the group  $K_{12}$  that would transform  $(\mathbf{S}_1^+ | \mathbf{n} | \mathbf{S}_3^-)$  into  $(\mathbf{S}_3^- | \mathbf{n} | \mathbf{S}_1^+)$ .

As we shall show in the next section, the symmetry group  $T_{12}(\mathbf{n})$  of a twin and the symmetry group  $T_{21}(\mathbf{n})$  of a reverse twin are equal,

$$T_{12}(\mathbf{n}) = T_{21}(\mathbf{n}). \quad (3.4.3.66)$$

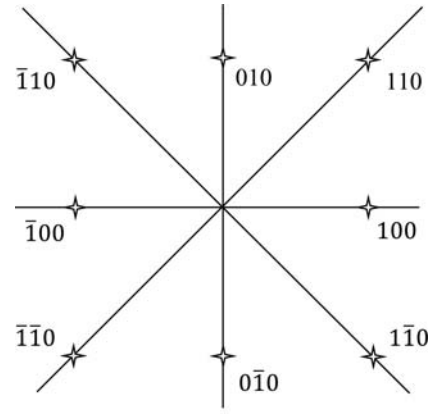
A sequence of repeating twins and reversed twins

$$\dots \mathbf{R}_1^+ | \mathbf{n} | \mathbf{R}_2^- | \mathbf{n} | \mathbf{R}_1^+ | \mathbf{n} | \mathbf{R}_2^- | \mathbf{n} | \mathbf{R}_1^+ | \mathbf{n} | \mathbf{R}_2^- | \mathbf{n} | \mathbf{R}_1^+ | \mathbf{n} | \mathbf{R}_2^- \dots \quad (3.4.3.67)$$

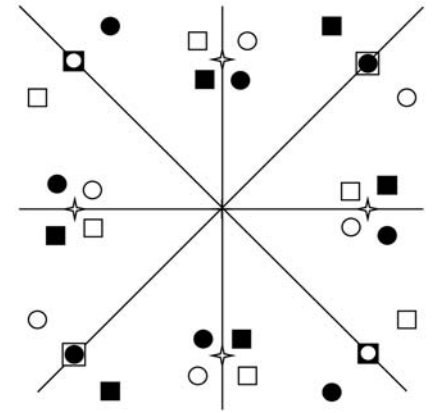
forms a *lamellar ferroelastic domain structure* that is very common in ferroelastic phases (see *e.g.* Figs. 3.4.1.1 and 3.4.1.4).

Similar considerations can be applied to the second equally deformed plane  $p'$  that is perpendicular to  $p$ . The two twins and corresponding compatible domain walls for the equally deformed plane  $p'$  have the symbols  $(\mathbf{R}_1^- | \mathbf{n}' | \mathbf{R}_2^+)$  and  $(\mathbf{R}_2^+ | \mathbf{n}' | \mathbf{R}_1^-)$ , and are also depicted in Fig. 3.4.3.8. The corresponding lamellar domain structure is

$$\dots \mathbf{R}_1^- | \mathbf{n}' | \mathbf{R}_2^+ | \mathbf{n}' | \mathbf{R}_1^- | \mathbf{n}' | \mathbf{R}_2^+ | \mathbf{n}' | \mathbf{R}_1^- | \mathbf{n}' | \mathbf{R}_2^+ | \mathbf{n}' | \mathbf{R}_1^- | \mathbf{n}' | \mathbf{R}_2^+ \dots \quad (3.4.3.68)$$



(a)



(b)

Fig. 3.4.3.9. Splitting of diffraction spots at a tetragonal-to-orthorhombic transition. (a) Fragment of the reciprocal lattice (stars) of the parent tetragonal phase. (b) Superposition of the reciprocal lattices of the four ferroelastic domains states in Fig. 3.4.3.8:  $\mathbf{R}_1^+$  (reciprocal lattice black squares),  $\mathbf{R}_1^-$  (reciprocal lattice black circles),  $\mathbf{R}_2^+$  (reciprocal lattice white squares) and  $\mathbf{R}_2^-$  (reciprocal lattice white circles).

Thus from one ferroelastic single-domain pair  $(\mathbf{R}_1, \mathbf{R}_2)$  depicted in the centre of Fig. 3.4.3.8 four different ferroelastic domain twins can be formed. It can be shown that these four twins have the same shear angle  $\omega$  and the same amount of shear  $s$ . They differ only in the direction of the shear.

Four disoriented domain states  $\mathbf{R}_1^-, \mathbf{R}_1^+$  and  $\mathbf{R}_2^-, \mathbf{R}_2^+$  that appear in the four domain twins considered above are related by lost operations (*e.g.* diagonal, vertical and horizontal reflections), *i.e.* they are crystallographically equivalent. This result can readily be obtained if we consider the stabilizer of a disoriented domain state  $\mathbf{R}_1^+$ , which is  $I_{4/mmm}(\mathbf{R}_1^+) = 2_z/m_z$ . Then the number  $n_a^{\text{dis}}$  of disoriented ferroelastic domain states is given by

$$n_a^{\text{dis}} = [G : I_g(\mathbf{R}_1^+)] = |4_z/m_z m_x m_{xy}| : |2_z/m_z| = 16 : 4 = 4. \quad (3.4.3.69)$$

All these domain states appear in ferroelastic polydomain structures that contain coexisting lamellar structures (3.4.3.67) and (3.4.3.68).

Disoriented domain states in ferroelastic domain structures can be recognized by diffraction techniques (*e.g.* using an X-ray precession camera). The presence of these four disoriented domain states results in splitting of the diffraction spots of the high-symmetry tetragonal phase into four or two spots in the orthorhombic ferroelastic phase. This splitting is schematically depicted in Fig. 3.4.3.9. For more details see *e.g.* Shmyt'ko *et al.* (1987), Rosová *et al.* (1993), and Rosová (1999).

### 3.4. DOMAIN STRUCTURES

Finally, we turn to *twin laws of ferroelastic domain twins with compatible domain walls*. In a ferroelastic twin, say  $(\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-)$ , there are just two possible *twinning operations* that interchange two ferroelastic domain states  $\mathbf{R}_1^+$  and  $\mathbf{R}_2^-$  of the twin: reflection through the plane of the domain wall ( $m_{xy}^*$  in our example) and  $180^\circ$  rotation with a rotation axis in the intersection of the domain wall and the plane of shear ( $2_{xy}^*$ ). These are the only transposing operations of the domain pair  $(\mathbf{R}_1, \mathbf{R}_2)$  that are preserved by the shear; all other transposing operations of the domain pair  $(\mathbf{R}_1, \mathbf{R}_2)$  are lost. (This is a difference from non-ferroelastic twins, where all transposing operations of the pair become twinning operations of a non-ferroelastic twin.)

Consider the twin  $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_3^-)$  in Fig. 3.4.3.8. By *non-trivial twinning operations* we understand transposing operations of the domain pair  $(\mathbf{S}_1^+, \mathbf{S}_3^-)$ , whereas *trivial twinning operations* leave invariant  $\mathbf{S}_1^+$  and  $\mathbf{S}_3^-$ . As we shall see in the next section, the union of trivial and non-trivial twinning operations forms a group  $T_{1+2-}(\mathbf{n})$ . This group, called the *symmetry group of the twin*  $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_3^-)$ , comprises all symmetry operations of this twin and we shall use it for designating the *twin law of the ferroelastic twin*, just as the group  $J_{ij}^*$  of the domain pair  $(\mathbf{S}_1, \mathbf{S}_j)$  specifies the twin law of a non-ferroelastic twin. This group  $T_{1+2-}(\mathbf{n})$  is a layer group (see Section 3.4.4.2) that keeps the plane  $p$  invariant, but for characterizing the twin law, which specifies the relation of domain states of two domains in the twin, one can treat  $T_{1+2-}(\mathbf{n})$  as an ordinary (dichromatic) point group  $T_{1+2-}(\mathbf{n})$ . Thus the twin law of the domain twin  $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_3^-)$  is designated by the group

$$T_{1+3-}(\mathbf{n}) = 2_{xy}^* m_{xy}^* m_z = T_{3-1+}(\mathbf{n}), \quad (3.4.3.70)$$

where (3.4.3.70) expresses the fact that a twin and the reversed twin have the same symmetry, see equation (3.4.3.66). We see that

this group coincides with the symmetry group  $J_{1+2-}$  of the single-domain pair  $(\mathbf{S}_1, \mathbf{S}_3)$  (see Fig. 3.4.3.1b).

The twin law of two twins  $(\mathbf{S}_1^-|\mathbf{n}'|\mathbf{S}_3^+)$  and  $(\mathbf{S}_3^+|\mathbf{n}'|\mathbf{S}_1^-)$  with the same equally deformed plane  $p'$  is expressed by the group

$$T_{1-3+}(\mathbf{n}') = m_z = T_{3-1+}(\mathbf{n}'), \quad (3.4.3.71)$$

which is different from the  $T_{1+3-}(\mathbf{n})$  of the twin  $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_3^-)$ .

Representative domain pairs of all orbits of ferroelastic domain pairs (Litvin & Janovec, 1999) are listed in two tables. Table 3.4.3.6 contains representative domain pairs for which compatible domain walls exist and Table 3.4.3.7 lists ferroelastic domain pairs where compatible coexistence of domain states is not possible. Table 3.4.3.6 contains, beside other data, for each ferroelastic domain pair the orientation of two equally deformed planes and the corresponding symmetries of the corresponding four twins which express two twin laws.

#### 3.4.3.6.4. Ferroelastic domain pairs with compatible domain walls, synoptic table

As we have seen, for each ferroelastic domain pair for which condition (3.4.3.54) for the existence of coherent domain walls is fulfilled, there exist two perpendicular equally deformed planes. On each of these planes two ferroelastic twins can be formed; these two twins are in a simple relation (one is a reversed twin of the other), have the same symmetry, and can therefore be represented by one of these twins. Then we can say that from one ferroelastic domain pair two different twins can be formed. Each of these twins represents a different ‘twin law’ that has arisen from the initial domain pair. All four ferroelastic twins can be described in terms of mechanical twinning with the same value of the shear angle  $\omega$ .

Table 3.4.3.6. Ferroelastic domain pairs and twins with compatible domain walls

$F_1$ : symmetry of domain state  $\mathbf{S}_1$ ;  $g_{ij}$ : switching operation,  $g_{ij}\mathbf{S}_1 = \mathbf{S}_j$ ;  $K(F_1, g_{ij})$ : twinning group, group extension of  $F_1$  by  $g_{ij}$ ; Axis  $\mathbf{h}$ : intersection of compatible walls; Equation: component  $B$  expressed as a function of strain components or lattice parameters (see end of table); Wall normals: coordinates of normals  $\mathbf{n}_1$  and  $\mathbf{n}_2$  of two perpendicular compatible walls, subscript  $e$ : wall is charged (see Explanation);  $\omega$ : obliquity, for numbers ( $n$ ) see end of table;  $\bar{J}_{ij}$ : extended layer-group symmetry of the twin and the wall;  $\bar{L}_{ij}^*$ : non-trivial twinning operation of the twin;  $T_{ij}$ : layer-group symmetry of the twin and the wall, twin law of the ferroelastic twin; Classification: classification of the twin and the wall (see Table 3.4.4.3).

$F_1$	$g_{ij}$	$K(F_1, g_{ij})$	Axis $\mathbf{h}$	Equation	Wall normals $\mathbf{n}$	$\omega$	$\bar{J}_{ij}$	$\bar{L}_{ij}^*$	$T_{ij}$	Classification
1	$2_z^*$	$2_z^*$	$[\bar{B}\bar{1}0]$	(a)	$[001]$ $[1B0]_e$	(1)	$2_z^*$ $2_z^*$	$2_z^*$	1 $2_z^*$	AR* SI
1	$m_z^*$	$m_z^*$	$[\bar{B}\bar{1}0]$	(a)	$[001]_e$ $[1B0]$	(1)	$m_z^*$ $m_z^*$	$m_z^*$	$m_z^*$ 1	SI AR*
$\bar{1}$	$m_z^*, 2_z^*$	$2_z^*/m_z^*$	$[\bar{B}\bar{1}0]$	(a)	$[001]$ $[1B0]$	(1)	$2_z^*/m_z^*$ $2_z^*/m_z^*$	$m_z^*$ $2_z^*$	$m_z^*$ $2_z^*$	SR SR
$2_z$	$2_x^*, 2_y^*$	$2_x^*2_y^*2_z$	$[001]$		$[100]$ $[010]$	(2)	$2_x^*2_y^*2_z$ $2_x^*2_y^*2_z$	$2_x^*$ $2_x^*$	$2_y^*$ $2_y^*$	SR SR
$2_z$	$m_x^*, m_y^*$	$m_x^*m_y^*2_z$	$[001]$		$[100]$ $[010]$	(2)	$m_x^*m_y^*2_z$ $m_x^*m_y^*2_z$	$m_x^*$ $m_x^*$	$m_y^*$ $m_y^*$	SR SR
$2_z$	$4_z^*, 4_z^{3*}$	$4_z^*$	$[001]$	(b)	$[1B0]$ $[B\bar{1}0]$	(3)	$2_z$ $2_z$		1 1	AR $\overline{AR}$
$2_z$	$\bar{4}_z^*, \bar{4}_z^{*3}$	$\bar{4}_z^*$	$[001]$	(b)	$[1B0]$ $[B\bar{1}0]$	(3)	$2_z$ $2_z$		1 1	AR $\overline{AR}$
$2_z$	$3_z, 6_z^5$	$6_z$	$[001]$	(c)	$[1B0]$ $[B\bar{1}0]$	(4)	$2_z$ $2_z$		1 1	AR $\overline{AR}$
	$3_z^2, 6_z$	$6_z$	$[001]$	(c)	$[1B0]$ $[B\bar{1}0]$	(4)	$2_z$ $2_z$		1 1	AR $\overline{AR}$
$2_z$	$\bar{3}_z^5, \bar{6}_z$	$6_z/m_z$	$[001]$	(c)	$[1B0]$ $[B\bar{1}0]$	(4)	$2_z$ $2_z$		1 1	AR $\overline{AR}$
	$\bar{3}_z, \bar{6}_z^5$	$6_z/m_z$	$[001]$	(c)	$[1B0]$ $[B\bar{1}0]$	(4)	$2_z$ $2_z$		1 1	AR $\overline{AR}$
$2_x$	$2_{xy}^*, 4_z$	$4_z2_x2_{xy}$	$[\bar{B}B2]$	(d)	$[110]$ $[11B]_e$	(5)	$2_{xy}^*$ $2_{xy}^*$	$2_{xy}^*$	1 $2_{xy}^*$	AR* SI
$2_x$	$m_{xy}^*, \bar{4}_z$	$\bar{4}_z2_xm_{xy}$	$[\bar{B}B2]$	(d)	$[110]_e$ $[11B]$	(5)	$m_{xy}^*$ $m_{xy}^*$	$m_{xy}^*$	$m_{xy}^*$ 1	SI AR*
$2_x$	$2_x^*, 3_z^2$	$3_z2_x$	$[\sqrt{3}B, B, \bar{4}]$	(e)	$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}1B]_e$	(6)	$2_x^*$ $2_x^*$	$2_x^*$	1 $2_x^*$	AR* SI