Table 3.4.3.7. *Ferroelastic domain pairs with no compatible domain walls*

F_1 is the symmetry of $\mathbf{S}_1$, g_{1j} is the switching operation, K_{1j} is the twinning group. Pair is the domain pair type, where ns is non-transposable simple and nm is non-transposable multiple (see Table 3.4.3.2). $v = z$, $p = [111]$, $q = [\bar{1}\bar{1}1]$, $r = [1\bar{1}\bar{1}]$, $s = [\bar{1}1\bar{1}]$ (see Table 3.4.2.5 and Fig. 3.4.2.3).

F_1	g_{1j}	K_{1j}	Pair
1	4_z	4_z	ns
1	$\bar{4}_z$	$\bar{4}_z$	ns
1	3_v	3_v	ns
1	$\bar{3}_v$	$\bar{3}_v$	ns
1	6_z	6_z	ns
1	$\bar{6}_z$	$\bar{6}_z$	ns
$\bar{1}$	4_z, 4_z^3	$4_z/m_z$	ns
$\bar{1}$	3_v, 3_v^2	$\bar{3}_v$	ns
$\bar{1}$	6_z, 6_z^5	$6_z/m_z$	ns
2_z	3_p, 3_p^2	$2_z 3_p$	nm
2_z	$\bar{3}_p$, $\bar{3}_p^5$	$m_z\bar{3}_p$	nm
2_{xy}	3_p, 3_p^2	$4_z 3_p 2_{xy}$	nm
2_{xy}	$\bar{3}_p$, $\bar{3}_p^5$	$m_z\bar{3}_p m_{xy}$	nm
m_z	3_p, 3_p^2	$m_z 3_p^2$	nm
m_{xy}	3_p, 3_p^2	$\bar{4}_z 3_p m_{xy}$	nm
m_{xy}	4_x, 4_x^3	$m_z\bar{3}_p m_{xy}$	nm
$2_z/m_z$	3_p, 3_p^2	$m_z\bar{3}_p$	nm
$2_{xy}/m_{xy}$	3_p, 3_p^2	$m_z\bar{3}_p m_{xy}$	nm
$2_x 2_y 2_z$	3_p, 3_p^2	$2_z 3_p$	ns
$2_x 2_y 2_z$	$\bar{3}_p$, $\bar{3}_p^5$	$m_z\bar{3}_p$	ns
$m_x m_y 2_z$	3_p, 3_p^2	$m_z\bar{3}_p$	nm
$m_x m_y m_z$	3_p, 3_p^2	$m_z\bar{3}_p$	ns

and $A'x_1 + B'x_2 + C'x_3 = 0$ [see equations (3.4.3.55)] pass through the origin of the Cartesian coordinate system of K_{1j} and have normal vectors $\mathbf{n}_1 = [ABC]$ and $\mathbf{n}_2 = [A'B'C']$. It is possible to find a plane with the same normal vector $[ABC]$ but not passing through the origin, *e.g.* $Ax_1 + Bx_2 + Cx_3 = 1$. Then parameters A, B and C can be interpreted as the reciprocal values of the oriented intercepts on the coordinate axes cut by this plane, $[x_1/(1/A)] + [x_2/(1/B)] + [x_3/(1/C)] = 1$. In analogy with Miller indices, the symbol (ABC) is used for expressing the orientation of a wall. However, parameters A, B and C are not Miller indices, since they are expressed in an orthonormal and not a crystallographic coordinate system. A left square bracket [in front of two equally deformed planes signifies that the two domain walls (domain twins) associated with one equally deformed plane are crystallographically equivalent (in K_{1j}) with two domain walls (twins) associated with the perpendicular equally deformed plane, *i.e.* all four compatible domain walls (domain twins) that can be formed from domain pair $(\mathbf{S}_1, \mathbf{S}_j)$ are crystallographically equivalent in K_{1j} (see Fig. 3.4.3.8).

The subscript e indicates that the wall carries a nonzero polarization charge, Div $\mathbf{P} \neq 0$. This can happen in ferroelectric domain pairs with spontaneous polarization not parallel to the axis of the pair. If one domain wall is charged then the perpendicular wall is not charged. In a few cases, polarization and/or orientation of the domain wall is not determined by symmetry; then it is not possible to specify which of the two walls is charged. In such cases, a subscript $e0$ or $0e$ indicates that one of the two walls is charged and the other is not.

ω: reference to an expression, given at the end of the table, in which the shear angle ω (in radians) is given as a function of the 'absolute' spontaneous strain components, defined in a matrix given above the equations.

$\bar{\mathsf{J}}_{1j}$: symmetry of the 'twin pair'. The meaning of this group and its symbol is explained in the next section. This group specifies the symmetry properties of a ferroelastic domain twin and the reversed twin with compatible walls of a given orientation and with domain states $\mathbf{S}_1^+, \mathbf{S}_j^-$ and $\mathbf{S}_1^+, \mathbf{S}_j^-$. This group can be used for designating a twin law of the ferroelastic domain twin.

$\underline{t}_{1j}^{\star}$: one non-trivial twinning operation of the twin $\mathbf{S}_1[ABC]\mathbf{S}_j$ and the wall. An underlined symbol with a star symbol signifies an operation that inverts the wall normal and exchanges the domain states (see the next section).

T_{1j}: layer-group symmetry of the ferroelastic domain twin and the reversed twin with compatible walls of a given orientation. Contains all trivial and non-trivial symmetry operations of the domain twin (see the next section).

Classification: symbol that specifies the type of domain twin and the wall. Five types of twins and domain walls are given in Table 3.4.4.3. The letter S denotes a symmetric domain twin (wall) in which the structures in two half-spaces are related by a symmetry operation of the twin, A denotes an asymmetric twin where there is no such relation. The letters R (reversible) and I (irreversible) signify whether a twin and reversed twin are, or are not, crystallographically equivalent in K_{1j}.

Example 3.4.3.7. The rhombohedral phase of perovskite crystals. Examples include PZN-PT and PMN-PT solid solutions (see *e.g.* Erhart & Cao, 2001) and $BaTiO_3$ below 183 K. The phase transition has symmetry descent $m\bar{3}m \supset 3m$.

In Table 3.4.2.7 we find that there are eight domain states and eight ferroelectric domain states. In this fully ferroelectric phase, domain states can be specified by unit vectors representing the direction of spontaneous polarization. We choose $\mathbf{S}_1 \equiv [111]$ with corresponding symmetry group $F_1 = 3_p m_{z\bar{y}}$.

From eight domain states one can form $7 \times 8 = 56$ domain pairs. These pairs can be divided into classes of equivalent pairs which are specified by different twinning groups. In column K_{1j} of Table 3.4.2.7 we find three twinning groups:

(i) The first twin law $\bar{3}_p^{\star} m_{x\bar{y}}$ characterizes a non-ferroelastic pair $(\mathrm{Fam}\bar{3}_p^{\star} m_{x\bar{y}} = \mathrm{Fam}3_p^{\star} m_{x\bar{y}})$ with inversion $\bar{1}$ as a twinning operation of this pair. A representative domain pair is $(\mathbf{S}_1, g_{12}\mathbf{S}_1 = \mathbf{S}_2) = ([111], [1\bar{1}\bar{1}])$, domain pairs consist of two domain states with antiparallel spontaneous polarization ('180° pairs'). Domain walls of low energy are not charged, *i.e.* they are parallel with the spontaneous polarization.

(ii) The second twinning group $K_{13} = \bar{4}3m$ characterizes a ferroelastic domain pair $(\mathrm{Fam}\bar{4}3m = m\bar{3}m \neq \mathrm{Fam}F_1 = \bar{3}_p m_{z\bar{y}})$. In Table 3.4.3.6, we find $g_{13}^{\star} = \underline{2}_x^{\star}$, which defines the representative pair $([111], [1\bar{1}\bar{1}])$ ('109° pairs'). Orientations of compatible domain walls of this domain pair are (100) and $(011)_e$ (this wall is charged). All equivalent orientations of these compatible walls will appear if all crystallographically equivalent pairs are considered.

(iii) The third twinning group $K_{14} = m\bar{3}m$ also represents ferroelastic domain pairs with representative pair $([111], m_x^{\star}[111]) = ([111], [\bar{1}11])$ ('71° pairs') and compatible wall orientations $(100)_e$ and (011). We see that for a given crystallographic orientation both charged and non-charged domain walls exist; for a given orientation the charge specifies to which class the domain wall belongs.

These conclusions are useful in deciphering the 'domain-engineered structures' of these crystals (Yin & Cao, 2000).

3.4.3.6.5. *Ferroelastic domain pairs with no compatible domain walls, synoptic table*

Ferroelastic domain pairs for which condition (3.4.3.54) for the existence of coherent domain walls is violated are listed in Table 3.4.3.7. All these pairs are non-transposable pairs. It is expected that domain walls between ferroelastic domain states would be stressed and would contain dislocations. Dudnik & Shuvalov (1989) have shown that in thin samples, where elastic stresses are reduced, 'almost coherent' ferroelastic domain walls may exist.

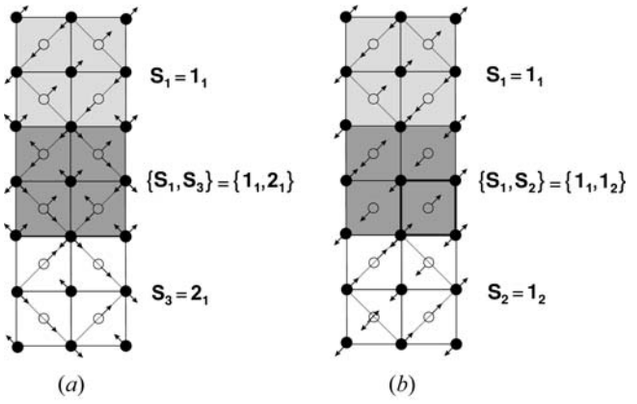

Fig. 3.4.3.10. Domain pairs in calomel. Single-domain states in the parent clamping approximation are those from Fig. 3.4.2.5. The first domain state of a domain pair is shown shaded in grey ('black'), the second domain state is colourless ('white'), and the domain pair of two interpenetrating domain states is shown shaded in dark grey. (*a*) Ferroelastic domain pair $(\mathsf{S}_1, \mathsf{S}_3)$ in the parent clamping approximation. This is a partially transposable domain pair. (*b*) Translational domain pair $(\mathsf{S}_1, \mathsf{S}_2)$. This is a completely transposable domain pair.

Example 3.4.3.8. Ferroelastic crystal of langbeinite. Langbeinite $K_2Mg_2(SO_4)_3$ undergoes a phase transition with symmetry descent $23 \supset 222$ that appears in Table 3.4.3.7. The ferroelastic phase has three ferroelastic domain states. Dudnik & Shuvalov (1989) found, in accord with their theoretical predictions, nearly linear 'almost coherent' domain walls accompanied by elastic stresses in crystals thinner than 0.5 mm. In thicker crystals, elastic stresses became so large that crystals were cracking and no domain walls were observed.

Similar effects were reported by the same authors for the partial ferroelastic phase of $CH_3NH_3Al(SO_4)_2{\cdot}12H_2O$ (MASD) with symmetry descent $\bar{3}m \supset mmm$, where ferroelastic domain walls were detected only in thin samples.

3.4.3.7. *Domain pairs in the microscopic description*

In the *microscopic description*, two microscopic domain states S_i and S_k with space-group symmetries $\mathcal{F}_i$ and $\mathcal{F}_k$, respectively, can form an ordered domain pair $(\mathsf{S}_i, \mathsf{S}_k)$ and an unordered domain pair $\{\mathsf{S}_i, \mathsf{S}_k\}$ in a similar way to in the continuum description, but one additional aspect has to be considered. The definition of the symmetry group $\mathcal{F}_{ik}$ of an ordered domain pair $(\mathsf{S}_i, \mathsf{S}_k)$,

$$\mathcal{F}_{ik} = \mathcal{F}_i \cap \mathcal{F}_k, \tag{3.4.3.72}$$

is meaningful only if the group $\mathcal{F}_{ik}$ is a space group with a three-dimensional translational subgroup (three-dimensional *twin lattice* in the classical description of twinning, see Section 3.3.8)

$$\mathcal{T}_{ik} = \mathcal{T}_i \cap \mathcal{T}_k, \tag{3.4.3.73}$$

where $\mathcal{T}_i$ and $\mathcal{T}_k$ are translation subgroups of $\mathcal{F}_i$ and $\mathcal{F}_k$, respectively. This condition is fulfilled if both domain states S_i and S_k have the same spontaneous strains, *i.e.* in non-ferroelastic domain pairs, but in ferroelastic domain pairs one has to suppress spontaneous deformations by applying the parent clamping approximation [see Section 3.4.2.2, equation (3.4.2.49)].

Example 3.4.3.9. Domain pairs in calomel. Calomel undergoes a non-equitranslational phase transition from a tetragonal parent phase to an orthorhombic ferroelastic phase (see Example 3.4.2.7 in Section 3.4.2.5). Four basic microscopic single-domain states are displayed in Fig. 3.4.2.5. From these states, one can form 12 non-trivial ordered single-domain pairs that can be partitioned (by means of double coset decomposition) into two orbits of domain pairs.

Representative domain pairs of these orbits are depicted in Fig. 3.4.3.10, where the first microscopic domain state S_i participating in a domain pair is displayed in the upper cell (light grey) and the second domain state S_j, $j = 2, 3$, in the lower white cell. The overlapping structure in the middle (dark grey) is a geometrical representation of the domain pair $\{\mathsf{S}_1, \mathsf{S}_j\}$.

The domain pair $\{\mathsf{S}_1, \mathsf{S}_3\}$, depicted in Fig. 3.4.3.10(*a*), is a ferroelastic domain pair in the parent clamping approximation. Then two overlapping structures of the domain pair have a common three-dimensional lattice with a common unit cell (the dotted square), which is the same as the unit cells of domain states S_1 and S_3.

Domain pair $\{\mathsf{S}_1, \mathsf{S}_2\}$, shown in Fig. 3.4.3.10(*b*), is a translational (antiphase) domain pair in which domain states S_1 and S_2 differ only in location but not in orientation. The unit cell (heavily outlined small square) of the domain pair $\{\mathsf{S}_1, \mathsf{S}_2\}$ is identical with the unit cell of the tetragonal parent phase (*cf.* Fig. 3.4.2.5).

The two arrows attached to the circles in the domain pairs represent exaggerated displacements within the wall.

Domain pairs represent an intermediate step in analyzing microscopic structures of domain walls, as we shall see in Section 3.4.4.

3.4.4. Domain twins and domain walls

3.4.4.1. *Formal description of simple domain twins and planar domain walls of zero thickness*

In this section, we examine crystallographic properties of planar compatible domain walls and simple domain twins. The symmetry of these objects is described by layer groups. Since this concept is not yet common in crystallography, we briefly explain its meaning in Section 3.4.4.2. The exposition is performed in the continuum description, but most of the results apply with slight generalizations to the microscopic treatment that is illustrated with an example in Section 3.4.4.7.

We shall consider a *simple domain twin* $\mathbf{T}_{12}$ that consists of two domains $\mathbf{D}_1$ and $\mathbf{D}_2$ which meet along a planar domain wall $\mathbf{W}_{12}$ of zero thickness. Let us denote by p a *plane of the domain wall*, in brief *wall plane* of $\mathbf{W}_{12}$. This plane is specified by Miller indices (hkl), or by a normal $\mathbf{n}$ to the plane which also defines the sidedness (plus and minus side) of the plane p. By *orientation of the plane p* we shall understand a specification which can, but may not, include the sidedness of p. If both the orientation and the sidedness are given, then the plane p divides the space into two half-spaces. Using the bra–ket symbols, mentioned in Section 3.4.3.6, we shall denote by $(\,|$ the half-space on the negative side of p and by $|\,)$ the half-space on the positive side of p.

A *simple twin* consists of two (theoretically semi-infinite) domains $\mathbf{D}_1$ and $\mathbf{D}_2$ with domain states $\mathbf{S}_1$ and $\mathbf{S}_2$, respectively, that join along a planar domain wall the orientation of which is specified by the wall plane p with normal $\mathbf{n}$. A symbol $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_2)$ specifies the domain twin unequivocally: domain $(\mathbf{S}_1|$, with domain region $(\,|$ filled with domain state $\mathbf{S}_1$, is on the negative side of p and domain $|\,\mathbf{S}_2)$ is on the positive side of p (see Fig. 3.4.4.1*a*).

If we were to choose the normal of opposite direction, *i.e.* $-\mathbf{n}$, the same twin would have the symbol $(\mathbf{S}_2|-\mathbf{n}|\mathbf{S}_1)$ (see Fig. 3.4.4.1*a*). Since these two symbols signify the same twin, we have the identity

$$(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_2) \equiv (\mathbf{S}_2|-\mathbf{n}|\mathbf{S}_1). \tag{3.4.4.1}$$

Thus, if we invert the normal $\mathbf{n}$ and simultaneously exchange domain states $\mathbf{S}_1$ and $\mathbf{S}_2$ in the twin symbol, we obtain an identical twin (see Fig. 3.4.4.1*a*). This identity expresses the fact that the