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_z3_p	nm
2_z	$\bar{3}_p$, $\bar{3}_p^5$	$m_z\bar{3}_p$	nm
2_{xy}	3_p, 3_p^2	$4_z3_p2_{xy}$	nm
2_{xy}	$\bar{3}_p$, $\bar{3}_p^5$	$m_z\bar{3}_pm_{xy}$	nm
m_z	3_p, 3_p^2	$m_z3_p^2$	nm
m_{xy}	3_p, 3_p^2	$\bar{4}_z3_pm_{xy}$	nm
m_{xy}	4_x, 4_x^3	$m_z\bar{3}_pm_{xy}$	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	$m_z\bar{3}_pm_{xy}$	nm
$2_x2_y2_z$	3_p, 3_p^2	2_z3_p	ns
$2_x2_y2_z$	$\bar{3}_p$, $\bar{3}_p^5$	$m_z\bar{3}_p$	ns
$m_xm_y2_z$	3_p, 3_p^2	$m_z\bar{3}_p$	nm
$m_xm_ym_z$	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 $F_1 = 3_pm_{z\bar{y}}$.

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 $(\mathrm{Fam}\bar{4}3m = m\bar{3}m \neq \mathrm{Fam}F_1 = \bar{3}_pm_{z\bar{y}})$. In Table 3.4.3.6, we find $g_{13}^{\star} = 2_x^{\star}$, which defines the representative pair $([111], [\bar{1}\bar{1}1])$ ('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.