

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)	$m_x^*m_y^*2_z$ $m_x^*m_y^*2_z$	$m_x^*$ $m_y^*$	$m_x^*$ $m_y^*$	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 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 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 AR
	$3_z^2, 6_z$	$6_z$	$[001]$	(c)	$[1B0]$ $[B\bar{1}0]$	(4)	$2_z$ $2_z$		1 1	AR 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 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 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

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

Table 3.4.3.6 (cont.)

$F_1$	$g_{1j}$	$K(F_1, g_{1j})$	Axis $\mathbf{h}$	Equation	Wall normals $\mathbf{n}$	$\omega$	$\bar{J}_{1j}$	$\bar{L}_{1j}^*$	$T_{1j}$	Classification
$2_x$	$m_x^*, \bar{3}_z^5$	$\bar{3}_z m_x$	$[\sqrt{3}B, B, \bar{4}]$	(e)	$[\bar{1}\sqrt{3}0]_e$ $[\sqrt{3}1B]$	(6)	$m_x^*$ $m_x^*$	$m_x^*$	$m_x^*$ 1	SI AR*
$2_x$	$2_{y'}^*, 6_z$	$6_z 2_x 2_y$	$[\bar{B}, \sqrt{3}B, \bar{4}]$	(f)	$[\sqrt{3}10]$ $[1\sqrt{3}B]_e$	(7)	$2_{y'}^*$ $2_{y'}^*$	$2_{y'}^*$	1 $2_{y'}^*$	AR* SI
$2_x$	$m_y^*, \bar{6}_z$	$\bar{6}_z 2_x m_y$	$[\bar{B}, \sqrt{3}B, \bar{4}]$	(f)	$[\sqrt{3}10]_e$ $[1\sqrt{3}B]$	(7)	$m_y^*$ $m_y^*$	$m_y^*$	$m_y^*$ 1	SI AR*
$2_{xy}$	$m_x^*, \bar{4}_z^3$	$\bar{4}_z m_x 2_{xy}$	$[0B\bar{1}]$	(g)	$[100]_e$ $[01B]$	(8)	$m_x^*$ $m_x^*$	$m_x^*$	$m_x^*$ 1	SI AR*
$m_z$	$m_x^*, 2_y^*$	$m_x^* 2_y^* m_z$	$[001]$		$[100]_e$ $[010]$	(2)	$m_x^* 2_y^* m_z$ $m_x^* 2_y^* m_z$	$m_x^*$	$m_x^* 2_y^* m_z$ $m_z$	SI AR*
$m_z$	$4_z, \bar{4}_z^3$	$4_z / m_z$	$[001]$	(b)	$[1B0]_{e0}$ $[B10]_{0e}$	(3)	$m_z$		$m_z$	AI AI
	$4_z^3, \bar{4}_z$	$4_z / m_z$	$[001]$	(b)	$[1B0]_{e0}$ $[B\bar{1}0]_{0e}$	(3)	$m_z$ $m_z$		$m_z$ $m_z$	AI AI
$m_z$	$3_z, \bar{6}_z^5$	$\bar{6}_z$	$[001]$	(c)	$[1B0]_{e0}$ $[B\bar{1}0]_{0e}$	(4)	$m_z$ $m_z$		$m_z$ $m_z$	AI AI
	$3_z^2, \bar{6}_z$	$\bar{6}_z$	$[001]$	(c)	$[1B0]_{e0}$ $[B10]_{0e}$	(4)	$m_z$ $m_z$		$m_z$ $m_z$	AI AI
$m_z$	$\bar{3}_z, 6_z^5$	$6_z / m_z$	$[001]$	(c)	$[1B0]_{e0}$ $[B\bar{1}0]_{0e}$	(4)	$m_z$ $m_z$		$m_z$ $m_z$	AI AI
	$\bar{3}_z^5, 6_z$	$6_z / m_z$	$[001]$	(c)	$[1B0]_{e0}$ $[B10]_{0e}$	(4)	$m_z$ $m_z$		$m_z$ $m_z$	AI AI
$m_x$	$m_{xy}^*, 4_z$	$4_z m_x m_{xy}$	$[\bar{B}B2]$	(d)	$[110]_e$ $[11B]$	(5)	$m_{xy}^*$ $m_{xy}^*$	$m_{xy}^*$	$m_{xy}^*$ 1	SI AR*
$m_x$	$2_{xy}^*, \bar{4}_z$	$\bar{4}_z m_x 2_{xy}$	$[\bar{B}B2]$	(d)	$[110]$ $[11B]_e$	(5)	$2_{xy}^*$ $2_{xy}^*$	$2_{xy}^*$	1 $2_{xy}^*$	AR* SI
$m_x$	$m_x^*, 3_z^2$	$3_z m_x$	$[\sqrt{3}B, B, \bar{4}]$	(e)	$[\bar{1}\sqrt{3}0]_e$ $[\sqrt{3}1B]$	(6)	$m_x^*$ $m_x^*$	$m_x^*$	$m_x^*$ 1	SI AR*
$m_x$	$2_{x'}^*, \bar{3}_z^5$	$\bar{3}_z m_x$	$[\sqrt{3}B, B, \bar{4}]$	(e)	$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}1B]_e$	(6)	$2_{x'}^*$ $2_{x'}^*$	$2_{x'}^*$	1 $2_{x'}^*$	AR* SI
$m_x$	$m_y^*, 6_z$	$6_z m_x m_y$	$[\bar{B}, \sqrt{3}B, \bar{4}]$	(f)	$[\sqrt{3}10]_e$ $[1\sqrt{3}B]$	(6)	$m_y^*$ $m_y^*$	$m_y^*$	$m_y^*$ 1	SI AR*
$m_x$	$2_{y'}^*, \bar{6}_z$	$\bar{6}_z m_x 2_{y'}$	$[\bar{B}, \sqrt{3}B, \bar{4}]$	(f)	$[\sqrt{3}10]$ $[1\sqrt{3}B]_e$	(6)	$2_{y'}^*$ $2_{y'}^*$	$2_{y'}^*$	1 $2_{y'}^*$	AR* SI
$m_{xy}$	$2_x^*, \bar{4}_z^3$	$\bar{4}_z 2_x m_{xy}$	$[0B\bar{1}]$	(h)	$[100]$ $[01B]_e$	(9)	$2_x^*$ $2_x^*$	$2_x^*$	1 $2_x^*$	AR* SI
$2_z / m_z$	$m_x^*, m_y^*$	$m_x^* m_y^* m_z$	$[001]$		$[100]$ $[010]$	(2)	$m_x^* m_y^* m_z$ $m_x^* m_y^* m_z$	$m_x^*$ $m_y^*$	$m_x^* 2_y^* m_z$ $2_x^* m_y^* m_z$	SR SR
$2_z / m_z$	$4_z^2, 4_z^{3*}$	$4_z^2 / m_z$	$[001]$	(b)	$[1B0]$ $[B\bar{1}0]$	(3)	$2_z / m_z$ $2_z / m_z$		$m_z$ $m_z$	AR AR
	$3_z, 6_z^5$	$6_z / m_z$	$[001]$	(c)	$[1B0]$ $[B10]$	(4)	$2_z / m_z$ $2_z / m_z$		$m_z$ $m_z$	AR AR
$2_z / m_z$	$3_z^2, 6_z$	$6_z / m_z$	$[001]$	(c)	$[1B0]$ $[B10]$	(4)	$2_z / m_z$ $2_z / m_z$		$m_z$ $m_z$	AR AR
	$2_x / m_x$	$m_{xy}^*, 4_z$	$4_z / m_x m_x m_{xy}$	$[\bar{B}B2]$	(d)	$[110]$ $[11B]$	(5)	$2_{xy}^* / m_{xy}^*$ $2_{xy}^* / m_{xy}^*$	$m_{xy}^*$ $2_{xy}^*$	$m_{xy}^*$ $2_{xy}^*$
$2_x / m_x$	$m_x^*, 3_z^2$	$\bar{3}_z m_x$	$[\sqrt{3}B, B, \bar{4}]$	(e)	$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}1B]$	(6)	$2_x^* / m_x^*$ $2_x^* / m_x^*$	$m_x^*$ $2_x^*$	$m_x^*$ $2_x^*$	SR SR
$2_x / m_x$	$m_y^*, 6_z$	$6_z / m_x m_x m_y$	$[\bar{B}, \sqrt{3}B, \bar{4}]$	(f)	$[\sqrt{3}10]$ $[1\sqrt{3}B]$	(6)	$2_y^* / m_y^*$ $2_y^* / m_y^*$	$m_y^*$ $2_y^*$	$m_y^*$ $2_y^*$	SR SR
$2_x 2_y 2_z$	$2_{xy}^*, 2_{xy}^*$	$4_z^2 2_x 2_{xy}$	$[001]$		$[110]$ $[110]$	(11)	$2_{xy}^* 2_{xy}^* 2_z$ $2_{xy}^* 2_{xy}^* 2_z$	$2_{xy}^*$ $2_{xy}^*$	$2_{xy}^*$ $2_{xy}^*$	SR SR
$2_x 2_y 2_z$	$m_{xy}^*, m_{xy}^*$	$\bar{4}_z^2 2_x m_{xy}^*$	$[001]$		$[110]$ $[110]$	(11)	$m_{xy}^* m_{xy}^* 2_z$ $m_{xy}^* m_{xy}^* 2_z$	$m_{xy}^*$ $m_{xy}^*$	$m_{xy}^*$ $m_{xy}^*$	SR SR
$2_x 2_y 2_z$	$2_{x'}^*, 2_{y'}^*$	$6_z 2_x 2_y$	$[001]$		$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}10]$	(10)	$2_{x'}^* 2_{y'}^* 2_z$ $2_{x'}^* 2_{y'}^* 2_z$	$2_{x'}^*$ $2_{x'}^*$	$2_{y'}^*$ $2_{y'}^*$	SR SR
$2_x 2_y 2_z$	$m_x^*, m_y^*$	$6_z / m_x m_x m_y$	$[001]$		$[\bar{1}\sqrt{3}0]$ $[\sqrt{3}10]$	(10)	$m_x^* m_y^* 2_z$ $m_x^* m_y^* 2_z$	$m_x^*$ $m_y^*$	$m_x^*$ $m_y^*$	SR SR
$2_{xy} 2_{xy} 2_z$	$m_x^*, m_y^*$	$\bar{4}_z^2 m_x 2_{xy}$	$[001]$		$[100]$ $[010]$	(13)	$m_x^* m_y^* 2_z$ $m_x^* m_y^* 2_z$	$m_x^*$ $m_y^*$	$m_x^*$ $m_y^*$	SR SR
$2_{xy} 2_{xy} 2_z$	$2_{xz}^*, 4_y$	$4_z 3_p 2_{xy}$	$[B2\bar{B}]$	(k)	$[101]$ $[\bar{1}B1]$	(12)	$2_{xz}^*$ $2_{xz}^*$	$2_{xz}^*$	1 $2_{xz}^*$	AR* SI
$2_{xy} 2_{xy} 2_z$	$m_{xz}^*, \bar{4}_y$	$m_z \bar{3}_p m_{xy}$	$[B2\bar{B}]$	(k)	$[101]$ $[\bar{1}B1]$	(12)	$m_{xz}^*$ $m_{xz}^*$	$m_{xz}^*$	$m_{xz}^*$ 1	SI AR*

### 3.4. DOMAIN STRUCTURES

Table 3.4.3.6 (cont.)


$F_1$	$g_{1j}$	$K(F_1, g_{1j})$	Axis $\mathbf{h}$	Equation	Wall normals $\mathbf{n}$	$\omega$	$\bar{J}_{1j}$	$\underline{J}_{1j}^*$	$\bar{T}_{1j}$	Classification
$m_x m_y 2_z$	$m_{xy}^*, m_{xy}^*$	$4_z^* m_x m_{xy}^*$	[001]		$\begin{bmatrix} [110] \\ [1\bar{1}0] \end{bmatrix}$	(11)	$\begin{matrix} m_{xy}^* m_{xy}^* 2_z \\ m_{xy}^* m_{xy}^* 2_z \end{matrix}$	$\begin{matrix} m_{xy}^* \\ m_{xy}^* \end{matrix}$	$\begin{matrix} m_{xy}^* \\ m_{xy}^* \end{matrix}$	SR SR
$m_x m_y 2_z$	$2_{xy}^*, 2_{xy}^*$	$4_z^* m_x 2_{xy}^*$	[001]		$\begin{bmatrix} [110] \\ [110] \end{bmatrix}$	(11)	$\begin{matrix} 2_{xy}^* 2_{xy}^* 2_z \\ 2_{xy}^* 2_{xy}^* 2_z \end{matrix}$	$\begin{matrix} 2_{xy}^* \\ 2_{xy}^* \end{matrix}$	$\begin{matrix} 2_{xy}^* \\ 2_{xy}^* \end{matrix}$	SR SR
$m_x m_y 2_z$	$m_x^*, m_y^*$	$6_z m_x m_y$	[001]		$\begin{bmatrix} [\bar{1}\sqrt{3}0] \\ [\sqrt{3}10] \end{bmatrix}$	(10)	$\begin{matrix} m_x^* m_y^* 2_z \\ m_x^* m_y^* 2_z \end{matrix}$	$\begin{matrix} m_x^* \\ m_y^* \end{matrix}$	$\begin{matrix} m_x^* \\ m_y^* \end{matrix}$	SR SR
$m_x m_y 2_z$	$2_x^*, 2_y^*$	$6_z / m_z m_x m_y$	[001]		$\begin{bmatrix} [\bar{1}\sqrt{3}0] \\ [\sqrt{3}10] \end{bmatrix}$	(10)	$\begin{matrix} 2_x^* 2_y^* 2_z \\ 2_x^* 2_y^* 2_z \end{matrix}$	$\begin{matrix} 2_x^* \\ 2_y^* \end{matrix}$	$\begin{matrix} 2_x^* \\ 2_y^* \end{matrix}$	SR SR
$m_x 2_y m_z$	$m_x^*, 2_y^*$	$6_z m_x 2_y$	[001]		$\begin{bmatrix} [\bar{1}\sqrt{3}0]_e \\ [\sqrt{3}10] \end{bmatrix}$	(10)	$\begin{matrix} m_x^* 2_y^* m_z \\ m_x^* 2_y^* m_z \end{matrix}$	$\begin{matrix} m_x^* \\ m_z \end{matrix}$	$\begin{matrix} m_x^* 2_y^* m_z \\ m_z \end{matrix}$	SI AR*
$2_x m_y m_z$	$m_{xy}^*, 2_{xy}^*$	$4_z / m_z m_x m_{xy}$	[001]		$\begin{bmatrix} [110] \\ [110]_e \end{bmatrix}$	(11)	$\begin{matrix} 2_{xy}^* m_{xy}^* m_z \\ 2_{xy}^* m_{xy}^* m_z \end{matrix}$	$\begin{matrix} m_{xy}^* \\ m_{xy}^* \end{matrix}$	$\begin{matrix} m_z \\ 2_{xy}^* m_{xy}^* m_z \end{matrix}$	AR* SI
$2_x m_y m_z$	$m_y^*, 2_x^*$	$6_z 2_x m_y$	[001]		$\begin{bmatrix} [\bar{1}\sqrt{3}0] \\ [\sqrt{3}10]_e \end{bmatrix}$	(10)	$\begin{matrix} 2_x^* m_y^* m_z \\ 2_x^* m_y^* m_z \end{matrix}$	$\begin{matrix} m_y^* \\ m_z \end{matrix}$	$\begin{matrix} m_z \\ 2_x^* m_y^* m_z \end{matrix}$	AR* SI
$2_x m_y m_z$	$m_x^*, 2_y^*$	$6_z / m_z m_x m_y$	[001]		$\begin{bmatrix} [\bar{1}\sqrt{3}0]_e \\ [\sqrt{3}10] \end{bmatrix}$	(10)	$\begin{matrix} m_x^* 2_y^* m_z \\ m_x^* 2_y^* m_z \end{matrix}$	$\begin{matrix} m_x^* \\ m_z \end{matrix}$	$\begin{matrix} m_x^* 2_y^* m_z \\ m_z \end{matrix}$	SI AR*
$m_{xy} m_{xy} 2_z$	$2_x^*, 2_y^*$	$4_z^* 2_x^* m_{xy}$	[001]		$\begin{bmatrix} [100] \\ [010] \end{bmatrix}$	(13)	$\begin{matrix} 2_x^* 2_y^* 2_z \\ 2_x^* 2_y^* 2_z \end{matrix}$	$\begin{matrix} 2_x^* \\ 2_y^* \end{matrix}$	$\begin{matrix} 2_x^* \\ 2_y^* \end{matrix}$	SR SR
$m_{xy} m_{xy} 2_z$	$m_{xz}^*, \bar{4}_y$	$4_z 3_p m_{xy}$	$[B2\bar{B}]$	(k)	$\begin{bmatrix} [101]_e \\ [\bar{1}B1] \end{bmatrix}$	(12)	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 1 \end{matrix}$	SI AR*
$m_{xy} m_{xy} 2_z$	$2_{xz}^*, 4_y$	$m_z \bar{3}_p m_{xy}$	$[B2\bar{B}]$	(k)	$\begin{bmatrix} [101] \\ [\bar{1}B1]_e \end{bmatrix}$	(12)	$\begin{matrix} 2_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} 1 \\ 2_{xz}^* \end{matrix}$	AR* SI
$m_{xy} 2_{xy} m_z$	$m_{xz}^*, 4_y$	$m_z \bar{3}_p m_{xy} (m_{xz}^*)$	$[B2\bar{B}]$	(k)	$\begin{bmatrix} [101]_e \\ [1B1] \end{bmatrix}$	(12)	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 1 \end{matrix}$	SI AR*
$m_{xy} 2_{xy} m_z$	$2_{xz}^*, \bar{4}_y$	$m_z \bar{3}_p m_{xy} (2_{xz}^*)$	$[B2\bar{B}]$	(k)	$\begin{bmatrix} [101] \\ [1B1]_e \end{bmatrix}$	(12)	$\begin{matrix} 2_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} 1 \\ 2_{xz}^* \end{matrix}$	AR* SI
$m_x m_y m_z$	$m_{xy}^*, m_{xy}^*$	$4_z^* / m_z m_x m_{xy}^*$	[001]		$\begin{bmatrix} [110] \\ [110] \end{bmatrix}$	(10)	$\begin{matrix} m_{xy}^* m_{xy}^* m_z \\ m_{xy}^* m_{xy}^* m_z \end{matrix}$	$\begin{matrix} m_{xy}^* \\ m_{xy}^* \end{matrix}$	$\begin{matrix} 2_{xy}^* m_{xy}^* m_z \\ m_{xy}^* 2_{xy}^* m_z \end{matrix}$	SR SR
$m_x m_y m_z$	$m_x^*, m_y^*$	$6_z / m_z m_x m_y$	[001]		$\begin{bmatrix} [\bar{1}\sqrt{3}0] \\ [\sqrt{3}10] \end{bmatrix}$	(10)	$\begin{matrix} m_x^* m_y^* m_z \\ m_x^* m_y^* m_z \end{matrix}$	$\begin{matrix} m_x^* \\ m_y^* \end{matrix}$	$\begin{matrix} m_x^* 2_y^* m_z \\ 2_x^* m_y^* m_z \end{matrix}$	SR SR
$m_{xy} m_{xy} m_z$	$m_{xz}^*, 4_y$	$m_z \bar{3}_p m_{xy}$	$[B2\bar{B}]$	(k)	$\begin{bmatrix} [101] \\ [1B1] \end{bmatrix}$	(12)	$\begin{matrix} 2_{xz}^* / m_{xz}^* \\ 2_{xz}^* / m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 2_{xz}^* \end{matrix}$	SR SR
$4_z$	$2_{xz}^*, 4_y$	$4_z 3_p 2_{xy}$	[010]		$\begin{bmatrix} [101] \\ [\bar{1}01]_e \end{bmatrix}$	(14)	$\begin{matrix} 2_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} 1 \\ 2_{xz}^* \end{matrix}$	AR* SI
$4_z$	$m_{xz}^*, \bar{4}_y$	$m_z \bar{3}_p m_{xy}$	[010]		$\begin{bmatrix} [101]_e \\ [\bar{1}01] \end{bmatrix}$	(14)	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 1 \end{matrix}$	SI AR*
$\bar{4}_z$	$m_{xz}^*, \bar{4}_y$	$\bar{4}_z 3_p m_{xy}$	[010]		$\begin{bmatrix} [101] \\ [101] \end{bmatrix}$	(14)	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 1 \end{matrix}$	SI AR*
$\bar{4}_z$	$2_{xz}^*, 4_y$	$m_z \bar{3}_p m_{xy}$	[010]		$\begin{bmatrix} [101] \\ [\bar{1}01]_e \end{bmatrix}$	(14)	$\begin{matrix} 2_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} 1 \\ 2_{xz}^* \end{matrix}$	AR* SI
$4_z / m_z$	$m_{xz}^*, 4_y$	$m_z \bar{3}_p m_{xy}$	[010]		$\begin{bmatrix} [101] \\ [\bar{1}01] \end{bmatrix}$	(14)	$\begin{matrix} 2_{xz}^* / m_{xz}^* \\ 2_{xz}^* / m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 2_{xz}^* \end{matrix}$	SR SR
$4_z 2_x 2_{xy}$	$2_{xz}^*, 2_{xz}^*$	$4_z 3_p 2_{xy}$	[010]		$\begin{bmatrix} [101] \\ [101] \end{bmatrix}$	(14)	$\begin{matrix} 2_{xz}^* 2_{xz}^* 2_y \\ 2_{xz}^* 2_{xz}^* 2_y \end{matrix}$	$\begin{matrix} 2_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} 2_{xz}^* \\ 2_{xz}^* \end{matrix}$	SR SR
$4_z 2_x 2_{xy}$	$m_{xz}^*, m_{xz}^*$	$m_z \bar{3}_p m_{xy}$	[010]		$\begin{bmatrix} [101] \\ [\bar{1}01] \end{bmatrix}$	(14)	$\begin{matrix} m_{xz}^* m_{xz}^* 2_y \\ m_{xz}^* m_{xz}^* 2_y \end{matrix}$	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	SR SR
$4_z m_x m_{xy}$	$m_{xz}^*, 2_{xz}^*$	$m_z \bar{3}_p m_{xy}$	[010]		$\begin{bmatrix} [101] \\ [\bar{1}01]_e \end{bmatrix}$	(14)	$\begin{matrix} 2_{xz}^* m_{xz}^* m_y \\ 2_{xz}^* m_{xz}^* m_y \end{matrix}$	$\begin{matrix} m_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} m_y \\ 2_{xz}^* m_{xz}^* m_y \end{matrix}$	AR* SI
$\bar{4}_z 2_x m_{xy}$	$m_{xz}^*, m_{xz}^*$	$\bar{4}_z 3_p m_{xy}$	[010]		$\begin{bmatrix} [101] \\ [101] \end{bmatrix}$	(14)	$\begin{matrix} m_{xz}^* m_{xz}^* 2_y \\ m_{xz}^* m_{xz}^* 2_y \end{matrix}$	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	SR SR
$\bar{4}_z m_x 2_{xy}$	$m_{xz}^*, 2_{xz}^*$	$m_z \bar{3}_p m_{xy}$	[010]		$\begin{bmatrix} [101] \\ [101] \end{bmatrix}$	(14)	$\begin{matrix} 2_{xz}^* m_{xz}^* m_y \\ 2_{xz}^* m_{xz}^* m_y \end{matrix}$	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	$\begin{matrix} m_y \\ 2_{xz}^* m_{xz}^* m_y \end{matrix}$	AR* SR
$\bar{4}_z 2_x m_{xy}$	$2_{xz}^*, 2_{xz}^*$	$m_z \bar{3}_p m_{xy}$	[010]		$\begin{bmatrix} [101] \\ [\bar{1}01] \end{bmatrix}$	(14)	$\begin{matrix} 2_{xz}^* 2_{xz}^* 2_y \\ 2_{xz}^* 2_{xz}^* 2_y \end{matrix}$	$\begin{matrix} 2_{xz}^* \\ 2_{xz}^* \end{matrix}$	$\begin{matrix} 2_{xz}^* \\ 2_{xz}^* 2_{xz}^* 2_y \end{matrix}$	SR SI
$4_z / m_z m_x m_{xy}$	$m_{xz}^*, m_{xz}^*$	$m_z \bar{3}_p m_{xy}$	[010]		$\begin{bmatrix} [101] \\ [101] \end{bmatrix}$	(14)	$\begin{matrix} m_{xz}^* m_{xz}^* m_y \\ m_{xz}^* m_{xz}^* m_y \end{matrix}$	$\begin{matrix} m_{xz}^* \\ m_{xz}^* \end{matrix}$	$\begin{matrix} m_{xz}^* 2_{xz}^* m_y \\ 2_{xz}^* m_{xz}^* m_y \end{matrix}$	SR SR
$3_p$	$2_x^*, 3_r$	$2_z 3_p$	$[01\bar{1}]$		$\begin{bmatrix} [100] \\ [011]_e \end{bmatrix}$	(15)	$\begin{matrix} 2_x^* \\ 2_x^* \end{matrix}$	$\begin{matrix} 2_x^* \\ 2_x^* \end{matrix}$	$\begin{matrix} 1 \\ 2_x^* \end{matrix}$	AR* SI
$3_p$	$m_x^*, \bar{3}_r$	$m_z \bar{3}_p$	$[01\bar{1}]$		$\begin{bmatrix} [100]_e \\ [011] \end{bmatrix}$	(15)	$\begin{matrix} m_x^* \\ m_x^* \end{matrix}$	$\begin{matrix} m_x^* \\ m_x^* \end{matrix}$	$\begin{matrix} m_x^* \\ 1 \end{matrix}$	SI AR*
$3_p$	$2_{xy}^*, 4_y$	$4_z 3_p 2_{xy}$	$[\bar{1}\bar{1}0]$		$\begin{bmatrix} [001]_e \\ [110] \end{bmatrix}$	(15)	$\begin{matrix} 2_{xy}^* \\ 2_{xy}^* \end{matrix}$	$\begin{matrix} 2_{xy}^* \\ 2_{xy}^* \end{matrix}$	$\begin{matrix} 2_{xy}^* \\ 1 \end{matrix}$	SI AR*
$3_p$	$m_{xy}^*, \bar{4}_y$	$\bar{4}_z 3_p m_{xy}$	$[\bar{1}\bar{1}0]$		$\begin{bmatrix} [001] \\ [110]_e \end{bmatrix}$	(15)	$\begin{matrix} m_{xy}^* \\ m_{xy}^* \end{matrix}$	$\begin{matrix} m_{xy}^* \\ m_{xy}^* \end{matrix}$	$\begin{matrix} 1 \\ m_{xy}^* \end{matrix}$	AR* SI

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

Table 3.4.3.6 (cont.)


$F_1$	$g_{1j}$	$K(F_1, g_{1j})$	Axis $\mathbf{h}$	Equation	Wall normals $\mathbf{n}$	$\omega$	$\bar{J}_{1j}$	$\bar{L}_{1j}^*$	$\bar{T}_{1j}$	Classification
$\bar{3}_p$	$m_x^*, 3_r$	$m_z \bar{3}_p$	$[01\bar{1}]$		$[100]$ $[011]$	(15)	$2_x^*/m_x^*$ $2_x^*/m_x^*$	$\underline{m}_x^*$ $\underline{2}_x^*$	$\underline{m}_x^*$ $\underline{2}_x^*$	SR SR
$\bar{3}_p$	$m_{xy}^*, 4_y$	$m_z \bar{3}_p m_{xy}$	$[\bar{1}\bar{1}0]$		$[001]$ $[110]$	(15)	$2_{xy}^*/m_{xy}^*$ $2_{xy}^*/m_{xy}^*$	$\underline{2}_{xy}^*$ $\underline{m}_{xy}^*$	$\underline{2}_{xy}^*$ $\underline{m}_{xy}^*$	SR SR
$3_p 2_{x\bar{y}}$	$2_x^*, 2_{yz}^*$	$4_z 3_p 2_{xy}$	$[01\bar{1}]$		$[100]$ $[011]$	(15)	$2_x^* 2_{yz}^* 2_{yz}^*$ $2_x^* 2_{yz}^* 2_{yz}^*$	$\underline{2}_{yz}^*$ $\underline{2}_x^*$	$\underline{2}_{yz}^*$ $\underline{2}_x^*$	SR SR
$3_p 2_{x\bar{y}}$	$m_x^*, m_{yz}^*$	$m_z \bar{3}_p m_{xy}$	$[01\bar{1}]$		$[100]$ $[011]$	(15)	$\underline{m}_x^* m_{yz}^* 2_{yz}^*$ $\underline{m}_x^* m_{yz}^* 2_{yz}^*$	$\underline{m}_x^*$ $\underline{m}_{yz}^*$	$\underline{m}_x^*$ $\underline{m}_{yz}^*$	SR SR
$3_p m_{x\bar{y}}$	$2_x^*, m_{yz}^*$	$4_z 3_p m_{xy}$	$[01\bar{1}]$		$[100]$ $[011]_e$	(15)	$\underline{m}_{yz}^* m_{yz}^* 2_x^*$ $\underline{m}_{yz}^* m_{yz}^* 2_x^*$	$\underline{m}_{yz}^*$	$\underline{m}_{yz}^*$ $\underline{m}_{yz}^* m_{yz}^* 2_x^*$	AR* SI
$3_p m_{x\bar{y}}$	$m_x^*, 2_{yz}^*$	$m_z \bar{3}_p m_{xy}$	$[01\bar{1}]$		$[100]_e$ $[011]$	(15)	$\underline{m}_x^* 2_{yz}^* m_{yz}^*$ $\underline{m}_x^* 2_{yz}^* m_{yz}^*$	$\underline{m}_x^*$	$\underline{m}_x^* 2_{yz}^* m_{yz}^*$ $\underline{m}_{yz}^*$	SI AR*
$\bar{3}_p m_{x\bar{y}}$	$m_x^*, m_{yz}^*$	$m_z \bar{3}_p m_{xy}$	$[01\bar{1}]$		$[100]$ $[011]$	(15)	$\underline{m}_x^* m_{yz}^* m_{yz}^*$ $\underline{m}_x^* m_{yz}^* m_{yz}^*$	$\underline{m}_x^*$ $\underline{m}_{yz}^*$	$\underline{m}_x^* 2_{yz}^* m_{yz}^*$ $\underline{2}_x^* m_{yz}^* m_{yz}^*$	SR SR

Expressions for obliquity  $\omega$  as a function of spontaneous strain components and lattice parameters

Expression	$\omega$ as a function of spontaneous strain components  $\begin{pmatrix} q & v & u \\ v & r & t \\ u & t & s \end{pmatrix}$	$\omega$ as a function of lattice parameters $a, b, c; \alpha = \angle(b; c), \beta = \angle(a; c), \gamma = \angle(a; b)$  
(1)	$\omega = 2\sqrt{t^2 + u^2}$	$\omega = \left  \arccos \frac{\sqrt{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma}}{\sin \gamma} \right $
(2)	$\omega = 2 v $	$\omega =  \pi/2 - \gamma $
(3)	$\omega = \sqrt{(q-r)^2 + 4v^2}$	$\omega = \left  \arcsin \frac{\sqrt{(2ab \cos \gamma)^2 + (b^2 - a^2)}}{b^2 - a^2} \right $
(4)	$\omega = \frac{\sqrt{3}}{2} \sqrt{(q-r)^2 + 4v^2}$	$\omega =  \pi/2 - \psi_1 - \psi_2 $  $\psi_1 = \text{arccotan} \frac{c^2(a^2 + b^2 - 2d^2) - (a^2 - b^2)^2 + D(a^2 - b^2 - d^2)}{(D - b^2 + d^2)\sqrt{4a^2d^2 - (a^2 - b^2 - d^2)^2}}$  $\psi_2 = \text{arccotan} \frac{b^2(a^2 - b^2) + d^2(a^2 - b^2) - D(a^2 - b^2 + d^2)}{(D - b^2 + d^2)\sqrt{4a^2d^2 - (a^2 - b^2 - d^2)^2}}$  $D = \sqrt{(a^2 - d^2)^2 - (a^2 - b^2)(b^2 - d^2)}$
(5)	$\omega = \sqrt{(q-r)^2 + 2t^2}$	$\omega = \left  \arcsin \frac{c^2(a^2 + b^2) \sin^2 \alpha - b^2(a + c \cos \alpha)(2Da + c \cos \alpha)}{\sqrt{c^2(a^2 + b^2) \sin^2 \alpha + b^2(a + c \cos \alpha)^2} \sqrt{c^2(a^2 + b^2) \sin^2 \alpha + b^2(2Da + c \cos \alpha)^2}} \right $  $D = \frac{ac \cos \alpha}{b^2 - a^2}$

### 3.4. DOMAIN STRUCTURES

Table 3.4.3.6 (cont.)

Expression	$\omega$ as a function of spontaneous strain components $\begin{pmatrix} q & v & u \\ v & r & t \\ u & t & s \end{pmatrix}$	$\omega$ as a function of lattice parameters $a, b, c; \alpha = \angle(b; c), \beta = \angle(a; c), \gamma = \angle(a; b)$  (*)
(6)	$\omega = \frac{\sqrt{3}}{2} \sqrt{(q-r)^2 + 4t^2}$	$\omega = \left  \arcsin \frac{(4a^2 - b^2) \left[ \left(1 - \frac{c \cos \beta}{a+b}\right) b \cos \beta - \frac{c}{2} \right] + \frac{3cb^2 \sin^2 \beta}{2}}{\sqrt{4a^2 - b^2(1 - 9 \sin^2 \beta)} \sqrt{(ac \sin \beta)^2 + (4a^2 - b^2) \left[1 - \frac{c \cos \beta}{a+b}\right] b - \frac{c \cos \beta}{2}}} \right $ (*)
(7)	$\omega = 2 t $	$\omega =  \pi/2 - \alpha $
(8)	$\omega = \frac{\sqrt{3}}{2} \sqrt{(q-r)^2 + 4t^2}$	$\omega = \left  \arcsin \frac{3b^2c - c(4a^2 - b^2) \sin^2 \alpha + 2b^2D\sqrt{4a^2 - b^2} \cos \alpha}{\sqrt{b^2 + (4a^2 - b^2) \sin^2 \alpha} \sqrt{9b^2c^2 + (4a^2 - b^2)(c^2 \sin^2 \alpha + 4b^2D^2) + 12b^2Dc\sqrt{4a^2 - b^2}}} \right $ (*)  $D = \frac{2ac \cos \alpha}{b^2 - a^2}$
(9)	$\omega = 2\sqrt{q^2 + f^2}$	$\omega = \left  \arccos \frac{\sqrt{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma} + 2 \cos \alpha \cos \beta \cos \gamma}{\sin \alpha} \right $
(10)	$\omega = \frac{\sqrt{3}}{2}  q - r $	$\omega = \left  \arcsin \frac{b^2 - a^2}{a\sqrt{2b^2 + a^2}} \right $
(11)	$\omega =  q - r $	$\omega = \left  \arcsin \frac{a^2 - b^2}{b^2 + a^2} \right $
(12)	$\omega = \sqrt{(q-s)^2 + 2v^2}$	$\omega = \left  \arcsin \frac{c^2(D \cos \gamma - 1) - a^2 \sin^2 \gamma}{\sqrt{c^2 + a^2 \sin^2 \gamma} \sqrt{4c^2(D^2 - D \cos \gamma) + c^2 + a^2 \sin^2 \gamma}} \right $  $D = \frac{2a^2 \cos \gamma}{c^2 - a^2}$
(13)	$\omega = 2 v $	$\omega =  \pi/2 - \gamma $
(14)	$\omega =  q - s $	$\omega = \left  \arcsin \frac{a^2 - c^2}{c^2 + a^2} \right $
(15)	$\omega = 2\sqrt{2} v $	$\omega = \left  \arcsin \frac{\sqrt{2} \cos \alpha}{1 + \cos \alpha} \right $

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

Table 3.4.3.6 (cont.)

Expressions for component  $B$  of wall normal as a function of spontaneous strain components and lattice parameters

Equation	$B$ as a function of spontaneous strain components $\begin{pmatrix} q & v & u \\ v & r & t \\ u & t & s \end{pmatrix}$	$B$ as a function of lattice parameters $a, b, c; \alpha = \angle(b; c), \beta = \angle(a; c), \gamma = \angle(a; b)$
(a)	$B = \frac{t}{u}$	
(b)	$B = \frac{2v + \sqrt{(q-r)^2 + 4v^2}}{q-r}$	$B = \frac{-2ab \cos \gamma + \sqrt{(2ab \cos \gamma)^2 + (b^2 - a^2)}}{b^2 - a^2}$
(c)	$B = \frac{(q-r) + 2\sqrt{3}v + 4\sqrt{(q-r)^2 + 4v^2}}{\sqrt{3}(r-q) + 2v}$	$B = 2 \frac{a^2 - c^2 - \sqrt{(a^2 - c^2)^2 - (a^2 - b^2)(b^2 - c^2)}}{a^2 - b^2} - 1$
(d)	$B = \frac{2t}{q-r}$	
(e)	$B = \frac{4t}{r-q}$	
(f)	$B = \frac{4t}{q-r}$	
(g)	$B = \frac{4t}{r-q}$	
(h)	$B = \frac{-u}{v}$	
(k)	$B = \frac{2v}{s-v}$	$B = \frac{2a^2 \cos \gamma}{c^2 - a^2}$

#### 3.4.3.6.4.1. Explanation of Table 3.4.3.6

Table 3.4.3.6 presents representative domain pairs of all classes of ferroelastic domain pairs for which compatible domain walls exist. The first five columns concern the domain pair. In subsequent columns, each row splits into two rows describing the orientation of two associated perpendicular equally deformed planes and the symmetry properties of the four domain twins that can be formed from the given domain pair. We explain the meaning of each column in detail.

The first three columns specify *domain pairs*.

$F_1$ : point-group symmetry (stabilizer in  $K_{1j}$ ) of the first domain state  $\mathbf{S}_1$  in a single-domain orientation.

$g_{1j}$ : switching operations (if available) that specify the domain pair ( $\mathbf{S}_1, \mathbf{S}_j = g_{1j}\mathbf{S}_1$ ). Subscripts  $x, y, z$  specify the orientation of the symmetry operations in the Cartesian coordinate system of  $K_{1j}$ . Subscripts  $x', y'$  and  $x'', y''$  denote a Cartesian coordinate system rotated about the  $z$  axis through 120 and 240°, respectively, from the Cartesian coordinate axes  $x$  and  $y$ . Diagonal directions are abbreviated:  $p = [111]$ ,  $q = [\bar{1}\bar{1}\bar{1}]$ ,  $r = [1\bar{1}\bar{1}]$ ,  $s = [\bar{1}\bar{1}1]$ . Where possible, mirror planes and 180° rotations are chosen such that the two perpendicular permissible walls have crystallographic orientations.

$K_{1j}$ : twinning group  $K(F_1, g_{1j})$  of the domain pair ( $\mathbf{S}_1, \mathbf{S}_j$ ). For the pair with  $F_1 = m_{xy}2_{xy}m_z$  and  $K = m\bar{3}m$ , where the twinning group does not specify the domain pair unambiguously, we add after  $K_{1j}$  in parentheses a switching operation  $2_{xz}^*$  or  $m_{xz}^*$  that defines the domain pair.

*Axis*: axis of ferroelastic domain pair around which single-domain states must be rotated to establish a contact along a compatible domain wall. This axis is parallel to the intersection of the two compatible domain walls given in the column *Wall normals* and its direction  $\mathbf{h}$  is defined by a vector product  $\mathbf{h} = \mathbf{n}_1 \times \mathbf{n}_2$  of normal vectors  $\mathbf{n}_1$  and  $\mathbf{n}_2$  of these walls. The letter  $B$  denotes components of  $\mathbf{h}$  which depend on spontaneous strain.

*Equation*: a reference to an expression, given at the end of the table, for the direction  $\mathbf{h}$  of the axis, where the component  $B$  in the column *Axis* is expressed as functions of spontaneous strain components, and the matrices above these expressions give the form of the 'absolute' spontaneous strain.

*Wall normals*: orientation of equally deformed planes. As explained above, each plane represents two mutually reversed compatible domain walls. Numbers or parameters  $B, C$  given in parentheses can be interpreted either as components of normal vectors to compatible walls or as intercepts analogous to Miller indices: Planes of compatible domain walls  $Ax_1 + Bx_2 + Cx_3 = 0$

### 3.4. DOMAIN STRUCTURES

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).  $v = z$ ,  $p = [111]$ ,  $q = [1\bar{1}1]$ ,  $r = [1\bar{1}\bar{1}]$ ,  $s = [11\bar{1}]$  (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
$m_{xy}$	$3_p, 3_p^2$	$4_z 3_p m_{xy}$	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,  $\text{Div } \mathbf{P} \neq 0$ . 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.

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

$\bar{J}_{1j}$ : 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.

$\bar{L}_{1j}$ : 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<sub>3</sub> 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  $\bar{3}_p^* m_{xy}$  characterizes a non-ferroelastic pair ( $\text{Fam} \bar{3}_p^* m_{xy} = \text{Fam} 3_p^* m_{xy}$ ) 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 ( $\text{Fam} \bar{4}3m = m\bar{3}m \neq \text{Fam} F_1 = \bar{3}_p m_{z\bar{y}}$ ). In Table 3.4.3.6, we find  $g_{13}^* = 2_x^*$ , 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)<sub>e</sub> (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  $([111], m_x^*[111]) = ([111], [111])$  ('71° pairs') and compatible wall orientations (100)<sub>e</sub> 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.