International Tables for Crystallography (2006). Vol. E, Table 5.2.5.2, p. 414.

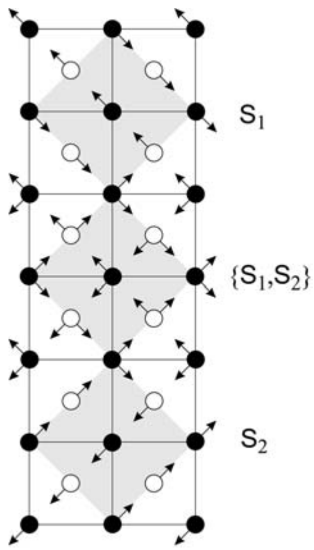

Fig. 5.2.5.6. The unordered domain pair between the two domain states.

The ferroic phase is orthorhombic with a space-group symmetry of the type *Cmcm* (D_{2h}^{17}), the conventional orthorhombic cell is based on vectors $\mathbf{a} = \mathbf{a}_t - \mathbf{b}_t$, $\mathbf{b} = \mathbf{a}_t + \mathbf{b}_t$, $\mathbf{c} = \mathbf{c}_t$ and contains two original cells. The conventional cell of the original tetragonal structure S and the cells of the four single domain states S_1, S_2, S_3 and S_4 are shaded in Fig. 5.2.5.5. The arrows represent spontaneous shifts (x, x), $(-x, x)$, $(-x, -x)$ and $(x, -x)$ of gravity centres of molecules. The two single domain states S_1 and S_3 have the symmetry *Amam* ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$); the other two single domain states S_2 and S_4 have the symmetry *Bbmm* ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$), where the Hermann–Mauguin symbols refer to the orthorhombic basis. There are two classes of domain pairs, represented by the pairs $\{\mathsf{S}_1, \mathsf{S}_2\}$ and $\{\mathsf{S}_1, \mathsf{S}_3\}$, which result in domain walls referred to as a ferroelastic domain wall and an antiphase boundary, respectively. We shall consider the first of these cases.

The two single domain states S_1, S_2 and the unordered pair $\{\mathsf{S}_1, \mathsf{S}_2\}$ are represented in Fig. 5.2.5.6. The symmetries of the single domain states and of both the ordered and unordered pair are given in Table 5.2.5.1, where subscripts indicate the orientation of symmetry elements with reference to the Cartesian basis and an asterisk denotes operations that exchange the single domain states.

We consider the domain walls of the orientation (100) with reference to the original tetragonal basis $(\mathbf{a}_t, \mathbf{b}_t, \mathbf{c}_t)$. This is the orientation with the Miller indices (110) with reference to the orthorhombic basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$. Consulting the scanning table No. 136 for the group $\mathcal{J}_{12} = P4^*_{2z}/m_z n_{xy} m^*_x$ ($\mathbf{b}_t/2$), we find the scanning group $Bm_y m_z m_x$ ($\mathbf{b}_t/2$) with reference to its conventional basis $(\mathbf{a}' = 2\mathbf{b}_t, \mathbf{b}' = \mathbf{c}_t, \mathbf{d} = 2\mathbf{a}_t)$, where $\mathbf{a}' = (-\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} + \mathbf{b})$. Applying the results of the scanning table with the shift by $\mathbf{b}_t/2 = \mathbf{a}'/4$, we obtain the sectional layer groups $\bar{\mathsf{J}}_{12}(0\mathbf{d})$ and $\bar{\mathsf{J}}_{12}(\frac{1}{4}\mathbf{d})$ and their floating subgroup $\bar{\mathsf{J}}_{12}(s\mathbf{d}) = \widehat{\mathsf{J}}_{12}(s\mathbf{d})$ (for $s \neq 0, \frac{1}{4}$). Analogously, for the space group $\mathcal{F}_{12}$, we obtain the sectional layer groups $\bar{\mathsf{F}}_{12}(0\mathbf{d})$ and $\bar{\mathsf{F}}_{12}(\frac{1}{4}\mathbf{d})$ and their floating subgroup $\bar{\mathsf{F}}_{12}(s\mathbf{d}) = \widehat{\mathsf{F}}_{12}(s\mathbf{d})$ (for $s \neq 0, \frac{1}{4}$). All these groups are collected in the Table 5.2.5.2 in two notations. In this table, with a specified basis, each standard symbol contains the same information as the optional symbol. Optional symbols contain subscripts which explicitly specify the orientations of symmetry elements with reference to the Cartesian coordinate system $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$, asterisks and underlines have the meaning specified above. The lattice symbol p means the common lattice $T(2\mathbf{b}_t, \mathbf{c}_t) = T(\mathbf{a}', \mathbf{b}')$ of all sectional layer groups and twin symmetries. The Hermann–Mauguin symbols are written with reference to the coordinate systems $(P + s\mathbf{d}; \mathbf{a}', \mathbf{b}', \mathbf{d})$.

The twin symmetry $\mathsf{T}_{12}(s\mathbf{d})$ is determined by the relation (5.2.5.7). This means, in practice, that we have to find the groups $\bar{\mathsf{J}}_{12}(s\mathbf{d})$, $\widehat{\mathsf{J}}_{12}(s\mathbf{d})$, $\bar{\mathsf{F}}_{12}(s\mathbf{d})$ and $\widehat{\mathsf{F}}_{12}(s\mathbf{d})$ from which we obtain the group $\mathsf{T}_{12}(s\mathbf{d})$. If tables of subgroups of layer groups were available, it would be sufficient to look up the subgroups which lie between $\bar{\mathsf{J}}_{12}(s\mathbf{d})$ and $\widehat{\mathsf{F}}_{12}(s\mathbf{d})$ and recognize the three groups $\bar{\mathsf{F}}_{12}(s\mathbf{d})$, $\widehat{\mathsf{J}}_{12}(s\mathbf{d})$ and $\mathsf{T}_{12}(s\mathbf{d})$.

Optional symbols facilitate this determination considerably. To get the twin symmetry $\mathsf{T}_{12}(s\mathbf{d})$, we look up the optional symbol for the group $\bar{\mathsf{J}}_{12}(s\mathbf{d})$ and eliminate elements that are either only underlined or that are only labelled by an asterisk. Or, *vice versa*, we leave only those elements that are not labelled at all or that are at the same time underlined and labelled by an asterisk. The resulting twin symmetries are given in the lower part of Table 5.2.5.2.

The implications of this symmetry analysis on the structure of domain walls at $0\mathbf{d}$ and $\frac{1}{4}\mathbf{d}$ are illustrated in Fig. 5.2.5.7. Shaded areas represent the domain states at infinity. The left-hand part of

Table 5.2.5.1. *Symmetries of domain states and domain pairs in a calomel crystal*

All groups in this table are expressed by their Hermann–Mauguin symbols with reference to orthorhombic basis $\mathbf{a} = \mathbf{a}_t - \mathbf{b}_t$, $\mathbf{b} = \mathbf{a}_t + \mathbf{b}_t$, $\mathbf{c} = \mathbf{c}_t$.

Object	Symmetry group	Type
Parent phase	$\mathcal{G} = I4/mmm$	D_{4h}^{17}
S_1	$\mathcal{F}_1 = Am_{x\bar{y}}a_{xy}m_z$ ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$)	D_{2h}^{17}
S_2	$\mathcal{F}_2 = Bb_{x\bar{y}}m_{xy}m_z$ ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$)	D_{2h}^{17}
$(\mathsf{S}_1, \mathsf{S}_2)$	$\mathcal{F}_{12} = Pn_{x\bar{y}}n_{xy}m_z$ ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$)	D_{2h}^{12}
$\{\mathsf{S}_1, \mathsf{S}_2\}$	$\mathcal{J}_{12} = P4^*_{2z}/m_z n_{xy} m^*_x$ ($\mathbf{b}_t/2$)	D_{4h}^{14} $[D_{2h}^{12}]$

Table 5.2.5.2. *Sectional layer groups of space groups $\mathcal{F}_{12}$ and $\mathcal{J}_{12}$ in the conventional basis $(\mathbf{a}' = 2\mathbf{b}_t, \mathbf{b}' = \mathbf{c}_t, \mathbf{d} = 2\mathbf{a}_t)$ of the scanning group $Bm_y m_z m_x$ and the respective twin symmetries*

		Location	Sectional layer group		
Space group	Plane (*hkl*)	$s\mathbf{d}$	$\mathcal{L}(s\mathbf{d})$	Standard symbol	Optional symbol
$\mathcal{F}_{12}$	(110)	$0\mathbf{d}$	$\bar{\mathsf{F}}_{12}(0\mathbf{d})$	$p12/m1$ ($\mathbf{b}_t/2$)	$p1\underline{2}_z/m_z1$ ($\mathbf{b}_t/2$)
		$\frac{1}{4}\mathbf{d}$	$\bar{\mathsf{F}}_{12}(\frac{1}{4}\mathbf{d})$	$p12/m1$	$p1\underline{2}_z/m_z1$
		$s\mathbf{d}$	$\bar{\mathsf{F}}_{12}(s\mathbf{d}) = \widehat{\mathsf{F}}_{12}$	$p1m1$	$p1m_z1$
$\mathcal{J}_{12}$		$0\mathbf{d}$	$\bar{\mathsf{J}}_{12}(0\mathbf{d})$	$pmmm$ ($\mathbf{b}_t/2$)	$p\underline{2}^*_y/m^*_y\ \underline{2}_z/m_z\ 2^*_x/\underline{m}^*_x$ ($\mathbf{b}_t/2$)
		$\frac{1}{4}\mathbf{d}$	$\bar{\mathsf{J}}_{12}(\frac{1}{4}\mathbf{d})$	$pmma$	$p\underline{2}^*_{1y}/m^*_y\ \underline{2}_z/m_z\ 2^*_x/\underline{a}^*_x$
		$s\mathbf{d}$	$\bar{\mathsf{J}}_{12}(s\mathbf{d}) = \widehat{\mathcal{J}}_{12}$	$pmm2$	$pm^*_y m_z 2^*_x$
Twin symmetries		Location	$\mathsf{T}_{12}(s\mathbf{d})$	Symmetry of the twin	
		$0\mathbf{d}$	$\mathsf{T}_{12}(0\mathbf{d})$	$p2mm$	$p\underline{2}^*_y m_z \underline{m}^*_x$
		$\frac{1}{4}\mathbf{d}$	$\mathsf{T}_{12}(\frac{1}{4}\mathbf{d})$	$p2_1ma$	$p\underline{2}^*_{1y} m_z \underline{a}^*_x$
		$s\mathbf{d}$	$\mathsf{T}_{12}(s\mathbf{d})$	$p1m1$	$p1m_z1$

references