Table 3.4.4.7. *Sectional layer groups and twin (wall) symmetries of the twin* (S_1|[100]; *s***d**|S_3) *in a calomel crystal*

Location *s***d**	$\overline{\mathcal{F}}_{13}$		$\overline{\mathcal{J}}_{13}$		T_{13}		
	Standard	Non-coordinate	Standard	Non-coordinate	Standard	Non-coordinate	Classification
$\frac{1}{4}$**d**, $\frac{3}{4}$**d**	$p12/m1$	$p\underline{2}_z/m_z$	$pmma$	$pm^\star_y m_z \underline{a}^\star_x$	$p2_1ma$	$p\underline{2}^\star_{1y} m_z \underline{a}^\star_x$	SR
0**d**, $\frac{1}{4}$**d**	$p12/m1$†	$p\underline{2}_z/m_z$†	$pmmm$†	$pm^\star_y m_z \underline{m}^\star_x$†	$p2mm$	$p\underline{2}^\star_y m_z \underline{m}^\star_x$	SR
*s***d**	$p1m1$	pm_z	$pmm2$	$p2^\star_x m^\star_y m_z$	$p1m1$	pm_z	AR*

† Shift of origin $\mathbf{b}_t/2$.

preserving and side-reversing operations, whereas for any other location *s***d** these layer groups are trivial (face) layer groups consisting of side-preserving operations only and are, therefore, also called *floating groups* in the direction **d** (*IT* E, 2010).

The wall (twin) symmetry T_{13} can be easily deduced from sectional layer groups $\overline{\mathcal{F}}_{13}$ and $\overline{\mathcal{J}}_{13}$: the floating group $\widehat{\mathcal{F}}_{13}$ is just the sectional layer group $\overline{\mathcal{F}}_{13}$ at a general location, $\widehat{\mathcal{F}}_{13} = \overline{\mathcal{F}}_{13}(s\mathbf{d}) = pm_z$. Two other generators in the group symbol of T_{13} are non-trivial twinning operations (underlined with a star) of $\overline{\mathcal{J}}_{13}$. The classification in the last column of Table 3.4.4.7 is defined in Table 3.4.4.3.

Local symmetry exerts constraints on possible displacements of the atoms within a wall. The site symmetry of atoms in a wall of zero thickness, or at the central plane of a finite-thickness domain wall, are defined by the layer group T_{13}. The site symmetry of the off-centre atoms at $0 < |\xi| < \infty$ are determined by floating group $\widehat{\mathcal{F}}_{13}$ and the limiting structures at $\xi \to -\infty$ and $\xi \to \infty$ by space groups $\mathcal{F}_1$ and $\mathcal{F}_3$, respectively. A reasonable condition that the displacements of atoms change continuously if one passes through the wall from $\xi \to -\infty$ to $\xi \to \infty$ allows one to deduce a qualitative picture of the displacements within a wall.

Symmetry groups of domain pairs, sectional layer groups and the twin symmetry have been derived in the parent clamping approximation (PCA) (see Section 3.4.2.5). As can be seen from Fig. 3.4.3.5, a relaxation process, accompanying a lifting of this approximation, consists of a simple shear (shear vector parallel to **q**) and an elongation (or contraction) in the domain wall along the shear direction (change of the vector $\overrightarrow{HB}_0$ into the vector $\overrightarrow{HB}_1^+$). These deformations influence neither the layer group T_{13} nor its floating group $\widehat{\mathcal{F}}_{13}$. Hence *the wall (twin) symmetry* T_{13} *derived in the parent clamping approximation expresses also the symmetry of a ferroelastic domain wall (twin) with nonzero spontaneous shear unless the simple shear is accompanied by a reshuffling of atoms or molecules in both domains*. This useful statement holds for any ferroelastic domain wall (twin).

A microscopic structure of the ferroelastic domain wall in two symmetrically prominent positions is depicted in Fig. 3.4.4.11. For better recognition, displacements of molecules are exaggerated and the changes of the displacement lengths are neglected. Since the symmetry of all groups involved contains a reflection m_z, the atomic shifts are confined to planes (001). It can be seen in the figure that when one moves through the wall in the direction [110] or [1$\bar{1}$0], the vector of the molecular shift experiences rotations through $\frac{1}{2}\pi$ about the $\mathbf{c}^t$ direction in opposite senses for the 'black' and 'white' molecules.

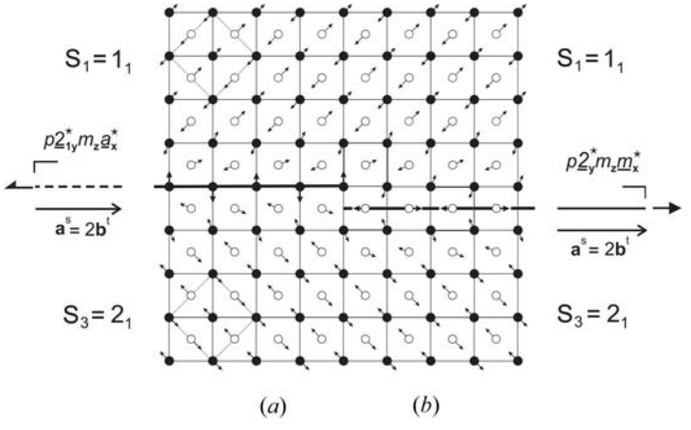

Fig. 3.4.4.11. Microscopic structure of a ferroelastic domain wall in calomel. (*a*) and (*b*) show a domain wall at two different locations with two different layer groups and two different structures of the central planes.

The 'black' molecules in the central layer at location $\frac{1}{4}$**d** or $\frac{3}{4}$**d** [wall (*a*) on the left-hand side of Fig. 3.4.4.11] exhibit nearly antiparallel displacements perpendicular to the wall. Strictly perpendicular shifts would represent 'averaged' displacements compatible with the layer symmetry $\overline{\mathcal{J}}_{13} = p\underline{2}^\star_{1y} m_z \underline{a}^\star_x$, which is, however, broken by a simple shear that decreases the symmetry to $\mathsf{T}_{13} = p\underline{2}^\star_{1y} m_z \underline{a}^\star_x$, which does not require perpendicular displacements of 'black' molecules.

The wall with central plane location 0**d** or $\frac{1}{4}$**d** (Fig. 3.4.4.11*b*) has symmetry $\mathsf{T}_{13} = p\underline{2}^\star_y m_z \underline{m}^\star_x$, which restricts displacements of 'white' molecules of the central layer to the y direction only; the 'averaged' displacements compatible with $\overline{\mathcal{J}}_{13} = pm^\star_y m_z \underline{m}^\star_x$ (origin shift $\mathbf{b}^t/2$) would have equal lengths of shifts in the $+y$ and $-y$ directions, but the relaxed central layer with symmetry $\mathsf{T}_{13} = p\underline{2}^\star_y m_z \underline{m}^\star_x$ allows unequal shifts in the $-y$ and $+y$ directions.

Walls (*a*) and (*b*) with two different prominent locations have different layer symmetries and different structures of the central layer. These two walls have extremal energy, but symmetry cannot decide which one has the minimum energy. The two walls have the same polar point-group symmetry $\underline{m}^\star_x \underline{2}^\star_y m_z$, which permits a spontaneous polarization along y.

Similar analysis of the displacement and ordering fields in domain walls has been performed for KSCN crystals (Janovec *et al.*, 1989), sodium superoxide NaO_2 (Zieliński, 1990) and for the simple cubic phase of fullerene C_{60} (Saint-Grégoire *et al.*, 1997).

3.4.5. Glossary

Note: the correspondence between contracted Greek indices and the Cartesian vector components used in Sections 3.1.3, in the present chapter and in the software *GI⋆KoBo*-1, is defined in the following way:

Cartesian components	11	22	33	23, 32	31, 13	12, 21
Contracted notation	1	2	3	4	5	6

In this designation, coefficients with contracted indices 4, 5, 6 appear two times, *e.g.* index 4 replaces yz in one coefficient and zy in the other coefficient. With this convention, the coefficients transform in tensor space as vector components, but some coefficients differ from the usual matrix notation (Voigt matrices) by numerical factors [see Section 1.1.4.10; Nye (1985); Sirotin & Shaskolskaya, Appendix E (1982)].

(*a*) Objects

Q_m	domain region
d	scanning vector (basis vector of a scanning group)
$\mathbf{D}_i(\mathbf{S}_k, Q_m)$	the ith domain, with domain state $\mathbf{S}_k$ in the mth domain region Q_m
$G\mathbf{S}_1$	G-orbit of principal single-domain states