International Tables for Crystallography (2006). Vol. E, Figure 5.2.5.5, p. 413.

group $\widehat{F}_{12}$. The $\underline{t}^*_{12}$ exchange the half-spaces because they invert the normal **n** and at the same time they exchange the domain states S_1 and S_2. As a result they leave the twin invariant, changing only the direction of the normal. These operations are called the *non-trivial symmetry operations of a domain twin*. If $\underline{t}^*_{12}$ is one such operation, then all these operations are contained in a coset $\underline{t}^*_{12}\widehat{F}_{12}$. Operations $\underline{s}_{12}$, called *the side-reversing operations*, exchange the half-spaces, leaving the domain states S_1 and S_2 invariant, and operations r^*_{12}, called *the state-reversing operations*, exchange the domain states S_1 and S_2, leaving the half-spaces invariant.

The symmetry group $T(S_1|\mathbf{n}; s\mathbf{d}|S_2)$, or in short T_{12}, of the twin $(S_1|\mathbf{n}; s\mathbf{d}|S_2)$ can therefore be generally be expressed as

$$T_{12} = \widehat{F}_{12} \cup \underline{t}^*_{12}\widehat{F}_{12}, \qquad (5.2.5.2)$$

where $\widehat{F}_{12}$ is a group of all trivial symmetry operations and $\underline{t}^*_{12}\widehat{F}_{12}$ is the coset of all non-trivial symmetry operations of the twin.

The group T_{12} is a layer group which can be deduced from four sectional layer groups of two space groups which describe the symmetry of two kinds of domain pairs formed from the domain states S_1 and S_2 (Janovec, 1972):

An *ordered domain pair* $(S_1, S_2) \neq (S_2, S_1)$ is an analogue of the dichromatic complex in which we keep track of the two components. The symmetry group of this pair must therefore leave invariant both domain states and is expressed as the intersection

$$\mathcal{F}_{12} = \mathcal{F}_1 \cap \mathcal{F}_2 = \mathcal{F}_1 \cap g_{12}\mathcal{F}_1 g_{12}^{-1} \qquad (5.2.5.3)$$

of symmetry groups $\mathcal{F}_1$ and $\mathcal{F}_2 = g_{12}\mathcal{F}_1 g_{12}^{-1}$ of the respective single domain states S_1 and S_2, where g_{12} is an operation transforming S_1 into S_2: $S_2 = g_{12}S_1$.

The sectional layer group $\bar{F}_{12}$ of the central plane with normal **n** and at a position $s\mathbf{d}$ under the action of the space group $\mathcal{F}_{12}$ is generally expressed as

$$\bar{F}_{12} = \widehat{F}_{12} \cup \underline{s}_{12}\widehat{F}_{12}, \qquad (5.2.5.4)$$

where the halving subgroup $\widehat{F}_{12}$ is the floating sectional layer group at a general position $s\mathbf{d}$. The operation $\underline{s}_{12}$ inverts the normal **n** and thus exchanges half-spaces on the left and right sides of the wall, where the left side is occupied by the state S_1 and the right side by the state S_2 in the initial twin. *These operations appear only at special positions of the central plane*. Since the half-spaces are occupied by domain states S_1 and S_2, their exchange is accompanied by an exchange of domain states on both sides of the wall. The operation $\underline{s}_{12}$ changes neither S_1 nor S_2 and hence it results in a *reversed domain twin* which has domain state S_2 on the left side and the domain state S_1 on the right side of the wall.

The *unordered domain pair* $\{S_1, S_2\} = \{S_2, S_1\}$ has the symmetry described by the group

$$\mathcal{J}_{12} = \mathcal{F}_{12} \cup j^*_{12}\mathcal{F}_{12}, \qquad (5.2.5.5)$$

where j^*_{12} is an operation that exchanges S_1 and S_2, $j^*_{12}S_1 = S_2$, $j^*_{12}S_2 = S_1$. Since for an unordered domain pair $\{S_1, S_2\} = \{S_2, S_1\}$, the symmetry operations of the left coset $j^*_{12}\mathcal{F}_{12}$ are also symmetry operations of the unordered domain pair $\{S_1, S_2\}$. If such an operation j^*_{12} and hence the whole coset $j^*_{12}\mathcal{F}_{12}$ of state-reversing operations exists, then the domain pair is called *transposable*. Otherwise $\mathcal{J}_{12} = \mathcal{F}_{12}$ and the domain pair is called *non-transposable*.

The sectional layer group of the space group $\mathcal{J}_{12}$ can therefore be generally written in the form

$$\bar{J}_{12} = \widehat{F}_{12} \cup r^*_{12}\widehat{F}_{12} \cup \underline{s}_{12}\widehat{F}_{12} \cup \underline{t}^*_{12}\widehat{F}_1. \qquad (5.2.5.6)$$

In the general case, the group $\bar{J}_{12}$ contains three halving subgroups which intersect at the subgroup $\widehat{F}_{12}$ of index four: the subgroup $\widehat{J}_{12} = \widehat{F}_{12} \cup r^*_{12}\widehat{F}_{12}$ is the floating subgroup of $\bar{J}_{12}$; the coset $r^*_{12}\widehat{F}_{12}$ is present if and only if the domain pair is transposable. The group $\bar{F}_{12} = \widehat{F}_{12} \cup \underline{s}_{12}\widehat{F}_{12}$ is the sectional layer group for the ordered domain pair defined above. Finally, the group $T_{12} = \widehat{F}_{12} \cup \underline{t}^*_{12}\widehat{F}_{12}$ is the symmetry group of the twin [see (5.2.5.2)]. Notice that it is itself not a sectional layer group of the space groups $\mathcal{F}_{12}$ and $\mathcal{J}_{12}$ involved unless $T_{12} = \widehat{F}_{12}$, which occurs in the case of a non-transposable domain pair and of a general position of the central plane.

Since the cosets can be set-theoretically expressed as differences of groups: $r^*_{12}\widehat{F}_{12} = \widehat{J}_{12} - \widehat{F}_{12}$ and $\underline{s}_{12}\widehat{F}_{12} = \bar{F}_{12} - \widehat{F}_{12}$, while $T_{12} = \bar{J}_{12} - [r^*_{12}\widehat{F}_{12} \cup \underline{s}_{12}\widehat{F}_{12}]$, we receive a compact set-theoretical expression for the symmetry group of the twin in terms of four sectional layer groups:

$$T_{12} = \bar{J}_{12} - [(\widehat{J}_{12} - \widehat{F}_{12}) \cup (\bar{F}_{12} - \widehat{F}_{12})]. \qquad (5.2.5.7)$$

Thus the symmetry group T_{12} of the twin can be expressed in terms of two sectional layer groups $\bar{F}_{12}$, $\bar{J}_{12}$ and their floating subgroups $\widehat{F}_{12}$, $\widehat{J}_{12}$, respectively. These four sectional layer groups can be found in the scanning tables.

As an illustrative example, we consider below a domain twin with a ferroelastic wall in the orthorhombic ferroelastic phase of the calomel crystal Hg_2Cl_2. Original analysis which includes the domain twin with antiphase boundary is given by Janovec & Zikmund (1993). Another analysis performed prior to the scanning tables is that of the domain twin in the KSCN crystal (Janovec *et al.*, 1989). Various cases of domain twins in fullerene C_{60} have also been analysed with the use of scanning tables (Janovec & Kopský, 1997; Saint-Grégoire, Janovec & Kopský, 1997).

Example: The parent phase of calomel has a tetragonal body-centred structure of space-group symmetry $I4/mmm$ (D^{17}_{4h}), where lattice points are occupied by calomel molecules which have the form of Cl–Hg–Hg–Cl chains along the c axis. The crystallographic coordinate system is defined by vectors of the conventional tetragonal basis $\mathbf{a}_t = a\mathbf{e}_x$, $\mathbf{b}_t = a\mathbf{e}_y$, $\mathbf{c}_t = c\mathbf{e}_z$ with reference to the Cartesian basis $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ and the origin P is chosen at the centre of gravity of one of the calomel molecules. The parent structure projected onto the $z = 0$ plane is depicted in the middle of Fig. 5.2.5.5, where full and empty circles denote the centres of gravity at the levels $z = 0$ and $z = c/2$, respectively.

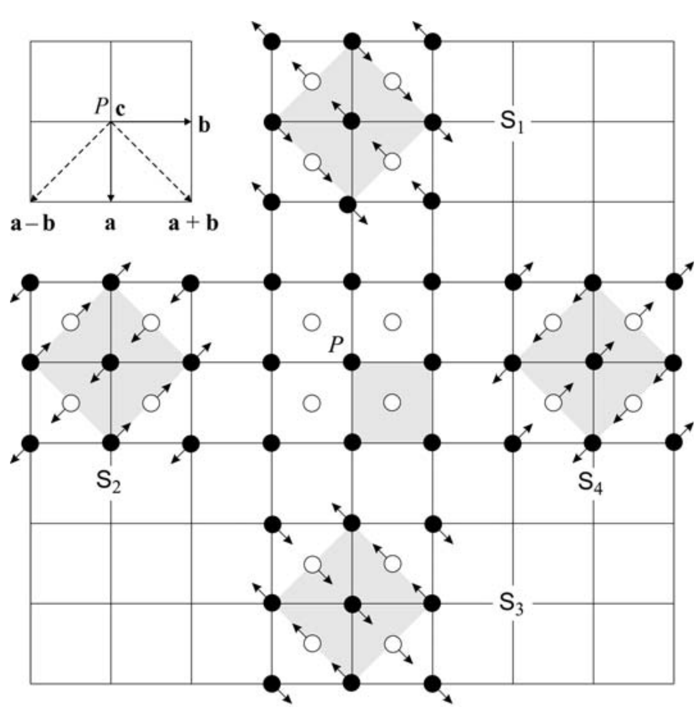

Fig. 5.2.5.5. The unit cell of the parent structure of calomel and the cells of four ferroic domain states.

references