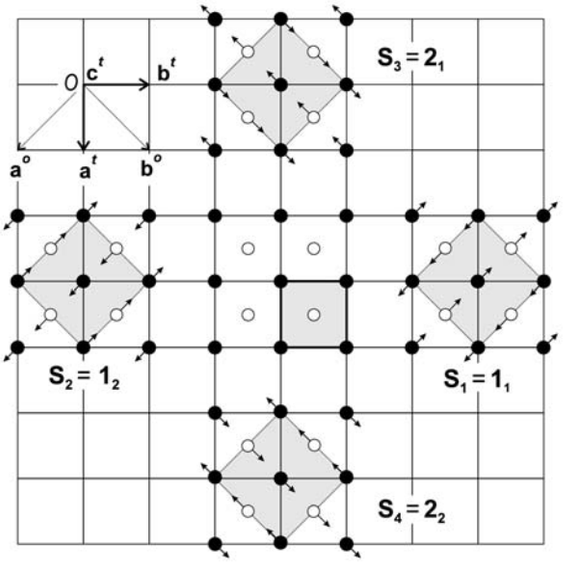


Fig. 3.4.2.5. Four basic single-domain states $S_1 = 1_1$, $S_2 = 1_2$, $S_3 = 2_1$, $S_4 = 2_2$ of the ferroic phase of a calomel ($Hg_2Cl_2$) crystal. Full • and empty ○ circles represent centres of gravity of $Hg_2Cl_2$ molecules at the levels $z = 0$ and $z = c/2$, respectively, projected onto the $z = 0$ plane. The parent tetragonal phase is depicted in the centre of the figure with a full square representing the primitive unit cell. Arrows are exaggerated spontaneous shifts of molecules in the ferroic phase. Dotted squares depict conventional unit cells of the orthorhombic basic domain states in the parent clamping approximation. If the parent clamping approximation is lifted, these unit cells would be represented by rectangles elongated parallel to the arrows.

this group is shifted by $\mathbf{a}^t/2$ or $\mathbf{b}$ with respect to the origin 0 of the group $\mathcal{G} = I4/mmm$.

Three more basic domain states $S_2$, $S_3$ and $S_4$ can be obtained, according to equation (3.4.2.44), from $S_1$ by applying representatives of the left cosets in the resolution of $\mathcal{G}$ [see equation (3.4.2.42)], for which one can find the expression

$$\mathcal{G} = \{1|000\}\mathcal{F}_1 \cup \{1|100\}\mathcal{F}_1 \cup \{4_z|000\}\mathcal{F}_1 \cup \{4_z^{\,3}|000\}\mathcal{F}_1. \quad (3.4.2.62)$$

All basic domain states $S_1$, $S_2$, $S_3$ and $S_4$ are depicted in Fig. 3.4.2.5. Domain states $S_1$ and $S_2$, and similarly $S_3$ and $S_4$, are related by lost translation $\mathbf{a}^t$ or $\mathbf{b}^t$. Thus the four basic domain states $S_1$, $S_2$, $S_3$ and $S_4$ can be partitioned into two translational subsets $\{S_1, S_2\}$ and $\{S_3, S_4\}$. Basic domain states forming one subset have the same value of the secondary macroscopic order parameter $\lambda$, which is in this case the difference $\varepsilon_{11} - \varepsilon_{22}$ of the components of a symmetric second-rank tensor $\varepsilon$, *e.g.* the permittivity or the spontaneous strain (which is zero in the parent clamping approximation).

This partition provides a useful labelling of basic domain states: $S_1 = 1_1$, $S_2 = 1_2$, $S_3 = 2_1$, $S_1 = 2_2$, where the first number signifies the ferroic (orientational) domain state and the subscript (translational index) specifies the basic domain state with the same ferroic domain state.

Symmetry groups (stabilizers in $\mathcal{G}$) of basic domain states can be calculated from a space-group version of equation (3.4.2.13):

$$\mathcal{F}_2 = \{1|100\}\mathcal{F}_2\{1|100\}^{-1} = \mathcal{F}_1;$$
$$\mathcal{F}_3 = \{4_z|000\}\mathcal{F}_2\{4_z|000\}^{-1} = Bbmm,$$

with the same conventional basis, and $\mathcal{F}_4 = \{1|100\}\mathcal{F}_3\{1|100\}^{-1} = \mathcal{F}_3$, where the origin of these groups is shifted by $\mathbf{a}^t/2$ or $\mathbf{b}$ with respect to the origin 0 of the group $\mathcal{G} = I4/mmm$.

In general, a space-group-symmetry descent $\mathcal{G} \supset \mathcal{F}_1$ can be performed in two steps:

(1) An equitranslational symmetry descent $\mathcal{G} \overset{t}{\supseteq} \mathcal{M}_1$, where $\mathcal{M}_1$ is the equitranslational subgroup of $\mathcal{G}$ (Hermann group), which is unequivocally specified by space group $\mathcal{G}$ and by the point group $F_1$ of the space group $\mathcal{F}_1$. The Hermann group $\mathcal{M}_1$ can be found in the software *GI★KoBo*-1 or, in some cases, in *IT* A (2005) under the entry 'Maximal non-isomorphic subgroups, type I'.

(2) An equiclass symmetry descent $\mathcal{M}_1 \overset{c}{\supseteq} \mathcal{F}_1$, which can be of three kinds [for more details see *IT* A (2005), Section 2.2.15]:

(i) Space groups $\mathcal{M}_1$ and $\mathcal{F}_1$ have the same conventional unit cell. These descents occur only in space groups $\mathcal{M}_1$ with centred conventional unit cells and the lost translations are some or all centring translations of the unit cell of $\mathcal{M}_1$. In many cases, the descent $\mathcal{M}_1 \supseteq \mathcal{F}_1$ can be found in the main tables of *IT* A (2005), under the entry 'Maximal non-isomorphic subgroups, type IIa'. Gadolinium molybdate belongs to this category.

(ii) The conventional unit cell of $\mathcal{M}_1$ is larger than that of $\mathcal{F}_1$. Some vectors of the conventional unit cell of $\mathcal{U}_1$ are multiples of that of $\mathcal{T}$. In many cases, the descent $\mathcal{M}_1 \supseteq \mathcal{F}_1$ can be found in the main tables of *IT* A (2005), under the entry 'Maximal non-isomorphic subgroups, type IIb'.

(iii) Space group $\mathcal{F}_1$ is an isomorphic subgroup of $\mathcal{M}_1$, *i.e.* both groups are of the same space-group type (with the same Hermann–Mauguin symbol) or of the enantiomorphic space-group type. Each space group has an infinite number of isomorphic subgroups. Maximal isomorphic subgroups of lowest index are tabulated in *IT* A (2005), under the entry 'Maximal non-isomorphic subgroups, type IIc'.

### 3.4.3. Domain pairs: domain twin laws, distinction of domain states and switching

Different domains observed by a single apparatus can exhibit different properties even though their crystal structures are either the same or enantiomorphic and differ only in spatial orientation. Domains are usually distinguished by their bulk properties, *i.e.* according to their domain states. Then the problem of domain distinction is reduced to the distinction of domain states. To solve this task, we have to describe in a convenient way the distinction of any two of all possible domain states. For this purpose, we use the concept of domain pair.

Domain pairs allow one to express the geometrical relationship between two domain states (the 'twin law'), determine the distinction of two domain states and define switching fields that may induce a change of one state into the other. Domain pairs also present the first step in examining domain twins and domain walls.

In this section, we define domain pairs, ascribe to them symmetry groups and so-called twinning groups, and give a classification of domain pairs. Then we divide domain pairs into equivalence classes ($G$-orbits of domain pairs) – which comprise domain pairs with the same inherent properties but with different orientations and/or locations in space – and examine the relation between $G$-orbits and twinning groups.

A qualitative difference between the coexistence of two domain states provides a basic division into non-ferroelastic and ferroelastic domain pairs. The synoptic Table 3.4.3.4 lists representatives of all $G$-orbits of *non-ferroelastic domain pairs*, contains information about the distinction of non-ferroelastic domain states by means of diffraction techniques and specifies whether or not important property tensors can distinguish between domain states of a non-ferroelastic domain pair. These data also determine the external fields needed to switch the first domain state into the second domain state of a domain pair. Synoptic Table 3.4.3.6 contains representative *ferroelastic domain pairs* of $G$-orbits of domain pairs for which there exist compatible (permissible) domain walls and gives for each representative pair the orientation of the *two compatible domain walls*, the expres-