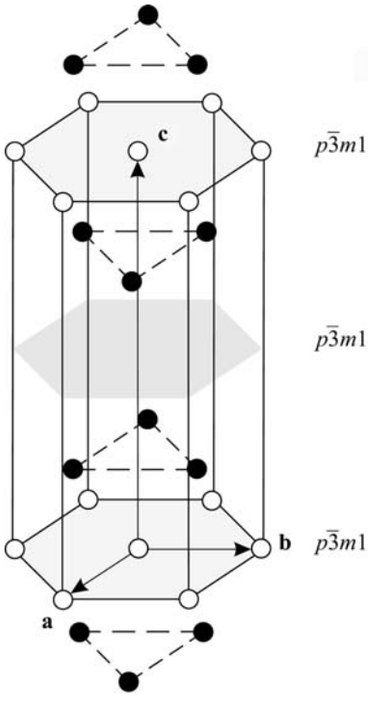

Fig. 5.2.5.1. The structure of cadmium iodide, CdI_2. The section planes of two orbits in special positions are distinguished by shading. The figure is drastically elongated in the c direction to exhibit the layer symmetries.

horizontal lines in the tables of orientation orbits and auxiliary bases. The orbit contains six orientations in groups of the Laue class $m\bar{3}$ (T_h) and 12 orientations in groups of the Laue class $m\bar{3}m$ (O_h). The orbit turns into a special orbit with fixed parameters for the special values $m = 1, n = 0$ in groups of both the Laue classes $m\bar{3}$ (T_h) and $m\bar{3}m$ (O_h). The scanning changes from monoclinic/inclined to orthorhombic in the Laue class $m\bar{3}$ (T_h), to tetragonal in the Laue class $m\bar{3}m$ (O_h). The symmetry of the orientation also increases to orthorhombic for special values $m = 1$, $n = 1$ in groups of the Laue class $m\bar{3}m$ (O_h).

The choice of bases for the three subsets is the same as in orthorhombic groups, where the orientations of subsets are separated into three different orbits and the auxiliary bases are expressed in terms of vectors of the conventional cubic basis for the centring types P and I. For the centring type F, the Miller indices differ in the original and auxiliary basis. In this case, we express the Miller indices with reference to the original basis as ($hk0$) and relate them to Miller indices ($mn0$) with reference to the auxiliary bases. These relations are the same as in the case of F-centring in orthorhombic groups, see relations (5.2.4.2) and (5.2.4.3).

Orientation orbit (*hhl*): The orbit contains 12 orientations which divide into three subsets corresponding to the three main cubic axes. In each of the subsets, one of the vectors of the conventional cubic basis is chosen as the vector $\widehat{\mathbf{b}}$ of the auxiliary basis. The orientations of the subsets are separated by horizontal lines across the table. The first subset corresponds to the vector $\mathbf{c}$ of the cubic basis and the orientations in this subset are the same as in the (*hhl*) orbit for tetragonal groups of the Laue class $4/mmm$ (D_{4h}). The orientations within each subset are further divided into two pairs of orientations to which correspond two different unique axes of the monoclinic scanning group. These subsets are again separated by horizontal lines across the last two columns. For the centring types P and I and for the first subset of orientations, the description of orientations and bases coincides with the description of the orbit (*hhl*) in tetragonal groups of the Laue class $4/mmm$ (D_{4h}) and centring types P and I, including the choice of auxiliary and conventional bases of scanning groups and relations between Miller indices h, l and m, n. For the other subsets of orientations, the data in tables are obtained by the cyclic permutation of vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$.

For the centring type F, orientation (*hhl*), we choose the auxiliary basis of the scanning group with the unique axis vectors $\widehat{\mathbf{c}} = (\mathbf{a} - \mathbf{b})/2$, $\widehat{\mathbf{b}} = \mathbf{c}$ and $\widehat{\mathbf{a}} = (\mathbf{a} + \mathbf{b})/2$, while for the orientation ($h\bar{h}l$), we choose $\widehat{\mathbf{c}} = (\mathbf{a} + \mathbf{b})/2$, $\widehat{\mathbf{b}} = \mathbf{c}$ and $\widehat{\mathbf{a}} = (\mathbf{a} - \mathbf{b})/2$. The bases for the remaining orientations are again obtained by the cyclic permutation of vectors of the conventional cubic basis.

Transformation of Miller indices: The straight line in which a plane (*hhl*) intersects with the plane ($1\bar{1}0$) has the direction of a vector $(\mathbf{a} + \mathbf{b})/2h - \mathbf{c}/l$ or of the vector $\mathbf{b}' = n\widehat{\mathbf{a}} - m\mathbf{c} = n(\mathbf{a} + \mathbf{b})/2 - m\mathbf{c}$. As these two vectors can differ only by a numerical factor, the pair $(2m, n)$ must be proportional to the pair (h, l) and we obtain the relations

$$h \text{ odd } \Rightarrow m = h, n = 2l; \quad h \text{ even } \Rightarrow m = h/2, n = l,$$

recorded at the bottom row of the orientation-orbit table for the centring type F.

For the special values $h = 1, l = 0$, this orbit turns into an orbit (110) with fixed parameters and an orthorhombic scanning group.

5.2.5. Applications

5.2.5.1. *Layer symmetries in crystal structures*

The following two examples show the use of layer symmetries in the description of crystal structures.

Example 1: Fig. 5.2.5.1 shows the crystal structure of cadmium iodide, CdI_2. The space group of this crystal is $P\bar{3}m1$, D^3_{3d} (No. 164). The anions form a hexagonal close packing of spheres and the cations occupy half of the octahedral holes, filling one of the alternate layers. In close-packing notation, the CdI_2 structure is:

A	C	B	C
I	Cd	I	void

From the scanning tables, we obtain for planes with the (0001) orientation and at heights $0\mathbf{c}$ or $\frac{1}{2}\mathbf{c}$ a sectional layer symmetry $p\bar{3}m1$ (L72), and for planes of this orientation at any other height a sectional layer symmetry $p3m1$ (L69).

The plane at height $0\mathbf{c}$ contains cadmium ions. This plane defines the orbit of planes of orientation (0001) located at points $P + n\mathbf{c}$, where $n \in Z$ (Z is the set of all integers). All these planes contain cadmium ions in the same arrangement (C layer filled with Cd).

The plane at height $\frac{1}{2}\mathbf{c}$ defines the orbit of planes of orientation (0001) located at points $P + (n + \frac{1}{2})\mathbf{c}$, where $n \in Z$. All these planes lie midway between A and B layers of iodine ions with the B layer below, the A layer above the plane. They contain only voids.

The planes at levels $\frac{1}{4}\mathbf{c}$ and $\frac{3}{4}\mathbf{c}$ contain B and A layers of iodine ions, respectively. These planes and all planes produced by translations $n\mathbf{c}$ from them belong to the same orbit because the operations $\bar{3}$ exchange the A and B layers.

Example 2: The space group of cadmium chloride, $CdCl_2$, is $R\bar{3}m$, D^5_{3d} (No. 166). Fig. 5.2.5.2 shows the structure of $CdCl_2$ in its triple hexagonal cell. The anions form a cubic close packing of spheres and the cations occupy half of the octahedral holes of each alternate layer. In close-packing notation, the $CdCl_2$ structure is:

A	C	B	A	C	B	A	C	B	A	C	B
Cl	Cd	Cl	void	Cl	Cd	Cl	void	Cl	Cd	Cl	void

We choose the origin at a cadmium ion and the hexagonal basis vectors $\mathbf{a}$, $\mathbf{b}$ as shown in Fig. 5.2.5.2. This corresponds to the obverse setting for which the scanning table is given in Part 6. The planes with the (0001) orientation at the heights $0\mathbf{c}$, $\frac{1}{6}\mathbf{c}$, $\frac{1}{3}\mathbf{c}$, $\frac{1}{2}\mathbf{c}$, $\frac{2}{3}\mathbf{c}$ and $\frac{5}{6}\mathbf{c}$ have a sectional layer group of the type $p\bar{3}m1$ (L72) and at any other height have a sectional layer group of the type $p3m1$ (L69).

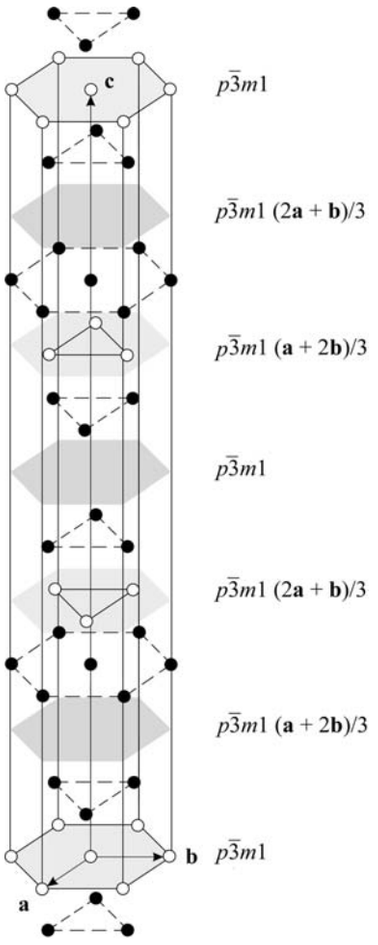

Fig. 5.2.5.2. The structure of cadmium chloride, CdI_2. The section planes of two orbits in special positions are distinguished by shading. Notice the different location of the sectional layer groups on different levels for the same orbit. The figure is drastically elongated in the *c* direction to exhibit the layer symmetries.

The scanning table also specifies the location of the sectional layer groups. The position along the *c* axis, where the basis vector $\mathbf{c} = \mathbf{d}$ specifies the scanning direction, is given by fractions of **d** or by *s***d** in the case of a general position. At the heights $0\mathbf{c}$ and $\frac{1}{2}\mathbf{c}$, the sectional layer group is the group $p\bar{3}m1$ (L72), while at the heights $\frac{1}{3}\mathbf{c}$ and $\frac{5}{6}\mathbf{c}$ it is the group $p\bar{3}m1$ $[(\mathbf{a}+2\mathbf{b})/3]$ (L72), and at the heights $\frac{2}{3}\mathbf{c}$ and $\frac{1}{6}\mathbf{c}$ it is the group $p\bar{3}m1$ $[(2\mathbf{a}+\mathbf{b})/3]$, (L72), where the vectors in brackets mean the shift of the group $p\bar{3}m1$ in space. The planes at the heights $0\mathbf{d}$, $\frac{1}{3}\mathbf{d}$ and $\frac{2}{3}\mathbf{d}$ belong to one translation orbit and the layers contain cadmium ions which are shifted relative to each other by the vectors $(\mathbf{a}+2\mathbf{b})/3$ and $(2\mathbf{a}+\mathbf{b})/3$. The planes at the heights $\frac{1}{2}\mathbf{d}$, $\frac{5}{6}\mathbf{d}$ and $\frac{1}{6}\mathbf{d}$ contain the voids and are located midway between layers of chlorine ions; they belong to another linear orbit and again are shifted relative to each other by the vectors $(\mathbf{a}+2\mathbf{b})/3$ and $(2\mathbf{a}+\mathbf{b})/3$.

5.2.5.2. *Interfaces in crystalline materials*

The scanning for the sectional layer groups is a procedure which finds applications in the theory of *bicrystals* and their *interfaces*. The first of these two terms was introduced in the study of grain boundaries (Pond & Bollmann, 1979; Pond & Vlachavas, 1983; Vlachavas, 1985; Kalonji, 1985). An *ideal bicrystal* is understood to be an aggregate of two semi-infinite crystals of identical structure, meeting at a common planar boundary called the *interface*, where one of the structures, occupying half-space on one side of the interface, is misoriented and/or displaced relative to the other structure occupying the other half-space. The word interface is a synonym for a boundary and interfaces considered here are *homophase interfaces*, in contrast with *heterophase interfaces*, where the two structures are different (Sutton & Balluffi, 1995).

An independent study of domain and twin boundaries (Janovec, 1981; Zikmund, 1984) resulted in a terminology parallel to that of the *bicrystallography*. The basic concept here is the *domain twin*, which is technically a particular case of a bicrystal. In this section, we use the terminology of bicrystals, giving the terminology of domain twins, used in the next section, parenthetically.

In both cases, the aim of the analysis is to determine the symmetry group of a bicrystal (domain twin), corresponding to a certain orientation and location of the interface (domain wall or twin boundary), which is a certain layer group.

The bicrystal (domain twin) is a conceivable real structure in space!

In the first step of the analysis, one constructs a *dichromatic complex* or *pattern* [(*unordered*) *domain pair*].

The dichromatic complex (domain pair) is not a real structure!

It is an abstract construction, a superposition of two infinite crystals which have the same structure, orientation and/or location as the two semi-infinite crystals of the bicrystal (domain twin) when extended to infinity. The two components are referred to as *black and white crystals* or *variants* (*single domain states*).

The symmetry group $\mathcal{J}$ of the dichromatic complex (domain pair) is the group of those Euclidean motions which either leave both black and white crystals (domain states) invariant or which exchange them. Planes of various orientations and locations, representing the interface, are then considered as transecting the dichromatic complex (domain pair). To each such plane there corresponds a sectional layer group $\bar{\mathsf{J}}$, the elements of which leave invariant the dichromatic pattern (domain pair) and the plane. A bicrystal (domain twin) is obtained by deleting from one side of the plane the atoms of one of the components of the dichromatic pattern (single domain states) and the atoms of the second component (single domain state) from the other side of the plane. The symmetry of the bicrystal (domain twin) is a layer group which contains those elements of the sectional layer group of the dichromatic pattern (domain pair) that satisfy one of the following two conditions:

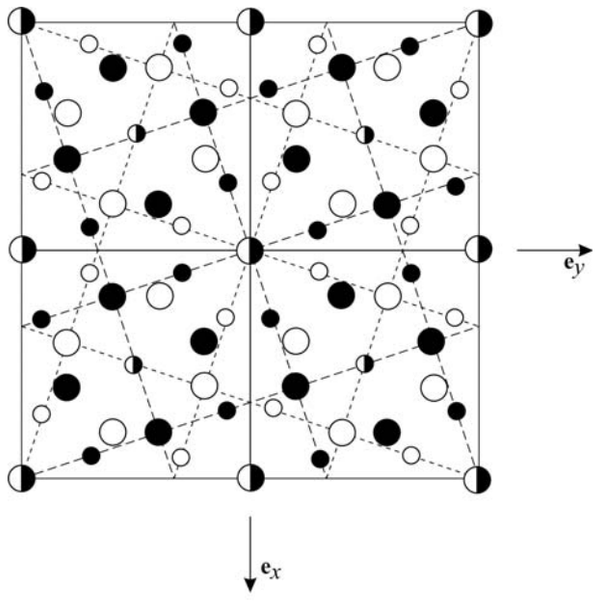

Fig. 5.2.5.3. A classical example of a bicrystal (Vlachavas, 1985).

(i) elements that leave invariant both the black and white crystals (both single domain states) and the normal to the plane;

(ii) elements that exchange the black and white crystals (single domain states) and invert the normal to the plane.

Example: Consider the bicrystal consisting of two face-centred cubic crystals misoriented by a rotation of 36.9° about the [001] direction. The corresponding dichromatic complex is shown in Fig. 5.2.5.3. The symmetry group of the complex is the space group $I4/mmm$, D_{4h}^{17} (No. 139).

Vlachavas (1985) has tabulated the symmetries of bicrystals arising when the above dichromatic complex is transected with planes of various orientations and locations. For planes of the orientation (001), given with reference to the tetragonal coordinate system shown in Fig. 5.2.5.3, Vlachavas lists

Orientation of plane	Position of plane		
(001)	$0, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}$	Other
Symmetry group of the bicrystal	$p422$	$p42_12$	$p411$

The position of the plane is given in terms of a fraction of the basis vector of the tetragonal c axis. The 'p' in the symbol of the symmetry groups of the bicrystal denotes all translations in the (001) plane.

From the subtable for the space group $I4/mmm$, D_{4h}^{17} (No. 139) in the scanning tables, Part 6, one finds

Orientation of plane	Position of plane		
(001)	$0, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}$	Other
Sectional layer group	$p4/mmm$	$p4/mmm$	$p4mm$

The symmetry group of the bicrystal is that subgroup of the corresponding sectional layer group consisting of all elements that satisfy one of the two conditions given above. For example, for the plane at position '0', the sectional layer group is $p4/mmm$ (L61). None of the mirror planes satisfies either of the conditions. The mirror plane perpendicular to [001] inverts the normal to the plane but leaves invariant both black and white crystals. The mirror planes perpendicular to [001] and [010] leave the normal to the plane invariant, but exchange the black and white crystals. The fourfold rotation satisfies condition (i), and the twofold rotations about auxiliary axes satisfy condition (ii). Consequently, from the sectional layer groups $p4/mmm$ (L61), $p4/nmm$ (L64) and $p4mm$ (L55) one obtains the respective symmetries of the bicrystal with different locations of interfaces: $p422$ (L53), $p42_12$ (L54) and $p4$ (L49), as listed by Vlachavas.

5.2.5.3. *The symmetry of domain twins and domain walls*

The symmetry of domain twins with planar coherent domain walls and the symmetry of domain walls themselves are also described by layer groups (see *e.g.* Janovec *et al.*, 1989), from which conclusions about the structure and tensorial properties of the domain walls can be deduced. The derivation of the layer symmetries of twins and domain walls is again facilitated by the scanning tables. As shown below, the symmetry of a twin is in general expressed through four sectional layer groups, where the central plane of the interface is considered as the section plane of an ordered and unordered domain pair. The relations between the symmetries and possible conclusions about the structure of the wall will be illustrated by an analysis of a domain twin in univalent mercurous halide (calomel) crystals.

A *twin* is a particular case of a bicrystal in which the relative orientation and/or displacement of the two components is not arbitrary; it is required that the operation that sends one of the components to the other is crystallographic. A *domain twin* is a special case where the structures S_1 and S_2 of the two components (*domains*) are distortions of a certain *parent* structure S, the symmetry of which is a certain space group $\mathcal{G}$, called the *parent group*. The parent structure S is either a real structure, the distortions of which are due to a structural phase transition, or it is a hypothetical structure. If the symmetry of one of the distorted structures S_1 is $\mathcal{F}_1$, then, from the coset decomposition

$$\mathcal{G} = \mathcal{F}_1 \cup g_2\mathcal{F}_1 \cup \ldots \cup g_p\mathcal{F}_1 \qquad (5.2.5.1)$$

we obtain $p = [\mathcal{G} : \mathcal{F}_1]$ equivalent distorted structures $\mathsf{S}_i = g_i\mathsf{S}_1$, $i = 1, 2, \ldots, p$, with symmetries $\mathcal{F}_i = g_i\mathcal{F}_1 g_i^{-1}$ which form a set of conjugate subgroups of $\mathcal{G}$.

Hence, a domain twin is always connected with a certain symmetry descent from a space group $\mathcal{G}$ to a set of conjugate subgroups $\mathcal{F}_i$. The distorted structures S_i are called the *single domain states*. A domain twin consists of two semi-infinite regions (half-spaces), called *domains*, separated by a planar interface called the *central plane*. The structures at infinite distance from this plane coincide with the domain states. The structure in the vicinity of the central plane is called the *domain wall*. The aim of the symmetry analysis is to determine the possible structure of the domain wall.

Basic theory: We consider a domain twin in which the domains are occupied by single domain states S_1 and S_2. To define the twin uniquely, we first observe that Miller indices (hkl) or corresponding normal $\mathbf{n}$ to the interface (central plane of the domain wall) define not only the orientation $V(\mathbf{a}', \mathbf{b}')$ of the wall but also its *sidedness*, so that one can distinguish between the two half-spaces. The normal $\mathbf{n}$ points from one of the half-spaces to the other while $-\mathbf{n}$ points in the opposite direction. The twin is then defined uniquely by the symbol $(\mathsf{S}_1|\mathbf{n}; s\mathbf{d}|\mathsf{S}_2) = (\mathsf{S}_1|(hkl); s\mathbf{d}|\mathsf{S}_2)$, which means that the domains are separated by the plane $(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ of orientation $V(\mathbf{a}', \mathbf{b}')$ and location $s\mathbf{d}$, where $\mathbf{d}$ is the scanning vector. The symbol also specifies that the normal $\mathbf{n}$ points from the half-space occupied by domain state S_1 to the half-space occupied by domain state S_2.

Now we consider the changes of the twin under the action of those isometries which leave the plane $(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ invariant. The action of such an isometry g on the twin is expressed by $g(\mathsf{S}_1|\mathbf{n}|\mathsf{S}_2) = (g\mathsf{S}_1|\widehat{g}\mathbf{n}|g\mathsf{S}_2)$, where $\widehat{g}$ is the *linear constituent* of the isometry g and $\widehat{g}\mathbf{n} = \pm\mathbf{n}$. Among these isometries, there are in general two kinds which define the symmetry of the twin and two which reverse the twin. The symbols for these four kinds of operations, their action on the initial twin $(\mathsf{S}_1|\mathbf{n}|\mathsf{S}_2)$, their graphical representation and the names of the resulting twins are as shown in Fig. 5.2.5.4.

An auxiliary notation has been introduced in which an asterisk labels operations that exchange the domain states and an underline labels operations that change the normal to the plane of the wall. To avoid misinterpretation (the symbolism is similar to that of the symmetry–antisymmetry groups), let us emphasize that neither the asterisk nor the underline have any meaning of an operation; they are just suitable labels which can be omitted without changing the meaning of general or specific symbols of the isometries. Operations with these labels mean the same as if the labels are dropped.

The operations f_{12} leave invariant the normal $\mathbf{n}$ as well as the states S_1 and S_2. Such operations are called the *trivial symmetry operations of a domain twin* and they constitute a certain layer

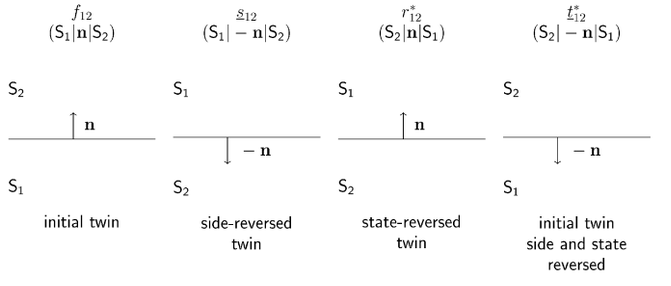

Fig. 5.2.5.4. The four types of operations on a twin.

group $\widehat{\mathsf{F}}_{12}$. 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 $\underline{t}^*_{12}\widehat{\mathsf{F}}_{12}$. 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 $\mathsf{T}(\mathsf{S}_1|\mathbf{n}; s\mathbf{d}|\mathsf{S}_2)$, or in short T_{12}, of the twin $(\mathsf{S}_1|\mathbf{n}; s\mathbf{d}|\mathsf{S}_2)$ can therefore be generally be expressed as

$$\mathsf{T}_{12} = \widehat{\mathsf{F}}_{12} \cup \underline{t}^*_{12}\widehat{\mathsf{F}}_{12}, \tag{5.2.5.2}$$

where $\widehat{\mathsf{F}}_{12}$ is a group of all trivial symmetry operations and $\underline{t}^*_{12}\widehat{\mathsf{F}}_{12}$ 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* $(\mathsf{S}_1, \mathsf{S}_2) \neq (\mathsf{S}_2, \mathsf{S}_1)$ 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

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

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: $\mathsf{S}_2 = g_{12}\mathsf{S}_1$.

The sectional layer group $\bar{\mathsf{F}}_{12}$ 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

$$\bar{\mathsf{F}}_{12} = \widehat{\mathsf{F}}_{12} \cup \underline{s}_{12}\widehat{\mathsf{F}}_{12}, \tag{5.2.5.4}$$

where the halving subgroup $\widehat{\mathsf{F}}_{12}$ 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* $\{\mathsf{S}_1, \mathsf{S}_2\} = \{\mathsf{S}_2, \mathsf{S}_1\}$ has the symmetry described by the group

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

where j^*_{12} is an operation that exchanges S_1 and S_2, $j^*_{12}\mathsf{S}_1 = \mathsf{S}_2$, $j^*_{12}\mathsf{S}_2 = \mathsf{S}_1$. Since for an unordered domain pair $\{\mathsf{S}_1, \mathsf{S}_2\} = \{\mathsf{S}_2, \mathsf{S}_1\}$, the symmetry operations of the left coset $j^*_{12}\mathcal{F}_{12}$ are also symmetry operations of the unordered domain pair $\{\mathsf{S}_1, \mathsf{S}_2\}$. 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

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

In the general case, the group $\bar{\mathsf{J}}_{12}$ contains three halving subgroups which intersect at the subgroup $\widehat{\mathsf{F}}_{12}$ of index four: the subgroup $\widehat{\mathsf{J}}_{12} = \widehat{\mathsf{F}}_{12} \cup r^*_{12}\widehat{\mathsf{F}}_{12}$ is the floating subgroup of $\bar{\mathsf{J}}_{12}$; the coset $r^*_{12}\widehat{\mathsf{F}}_{12}$ is present if and only if the domain pair is transposable. The group $\bar{\mathsf{F}}_{12} = \widehat{\mathsf{F}}_{12} \cup \underline{s}_{12}\widehat{\mathsf{F}}_{12}$ is the sectional layer group for the ordered domain pair defined above. Finally, the group $\mathsf{T}_{12} = \widehat{\mathsf{F}}_{12} \cup \underline{t}^*_{12}\widehat{\mathsf{F}}_{12}$ 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 $\mathsf{T}_{12} = \widehat{\mathsf{F}}_{12}$, 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: $r^*_{12}\widehat{\mathsf{F}}_{12} = \widehat{\mathsf{J}}_{12} - \widehat{\mathsf{F}}_{12}$ and $\underline{s}_{12}\widehat{\mathsf{F}}_{12} = \bar{\mathsf{F}}_{12} - \widehat{\mathsf{F}}_{12}$, while $\mathsf{T}_{12} = \bar{\mathsf{J}}_{12} - [r^*_{12}\widehat{\mathsf{F}}_{12} \cup \underline{s}_{12}\widehat{\mathsf{F}}_{12}]$, we receive a compact set-theoretical expression for the symmetry group of the twin in terms of four sectional layer groups:

$$\mathsf{T}_{12} = \bar{\mathsf{J}}_{12} - [(\widehat{\mathsf{J}}_{12} - \widehat{\mathsf{F}}_{12}) \cup (\bar{\mathsf{F}}_{12} - \widehat{\mathsf{F}}_{12})]. \tag{5.2.5.7}$$

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

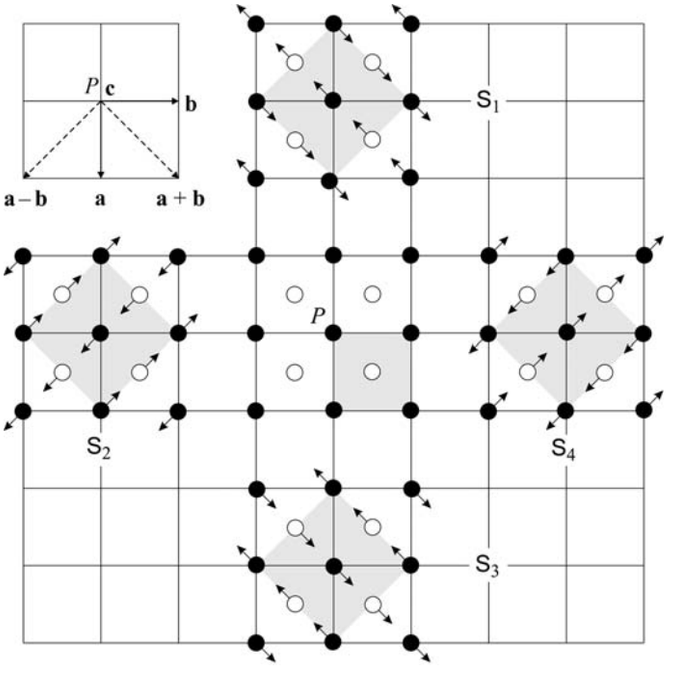

Fig. 5.2.5.5. The unit cell of the parent structure of calomel and the cells of four ferroic domain states.

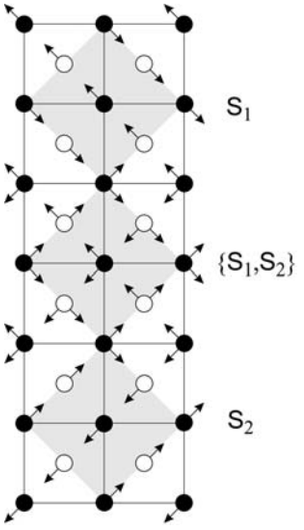

Fig. 5.2.5.6. The unordered domain pair between the two domain states.

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.

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} $[D_{2h}^{12}]$

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 5.2.5.2. *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*

Space group	Plane (*hkl*)	Location	Sectional layer group		
		$s\mathbf{d}$	$\mathcal{L}(s\mathbf{d})$	Standard symbol	Optional symbol
$\mathcal{F}_{12}$	(110)	$0\mathbf{d}$	$\bar{\mathsf{F}}_{12}(0\mathbf{d})$	$p12/m1$ ($\mathbf{b}_t/2$)	$p1\underline{2}_z/m_z1$ ($\mathbf{b}_t/2$)
		$\frac{1}{4}\mathbf{d}$	$\bar{\mathsf{F}}_{12}(\frac{1}{4}\mathbf{d})$	$p12/m1$	$p1\underline{2}_z/m_z1$
		$s\mathbf{d}$	$\bar{\mathsf{F}}_{12}(s\mathbf{d}) = \widehat{\mathsf{F}}_{12}$	$p1m1$	$p1m_z1$
$\mathcal{J}_{12}$		$0\mathbf{d}$	$\bar{\mathsf{J}}_{12}(0\mathbf{d})$	$pmmm$ ($\mathbf{b}_t/2$)	$p2_y^*/m_y^*\ \underline{2}_z/m_z\ 2_x^*/\underline{m}_x^*$ ($\mathbf{b}_t/2$)
		$\frac{1}{4}\mathbf{d}$	$\bar{\mathsf{J}}_{12}(\frac{1}{4}\mathbf{d})$	$pmma$	$p\underline{2}_{1y}^*/m_y^*\ \underline{2}_z/m_z\ 2_x^*/\underline{a}_x^*$
		$s\mathbf{d}$	$\bar{\mathsf{J}}_{12}(s\mathbf{d}) = \widehat{\mathcal{J}}_{12}$	$pmm2$	$pm_y^*m_z2_x^*$
Twin symmetries		Location	$\mathsf{T}_{12}(s\mathbf{d})$	Symmetry of the twin	
		$0\mathbf{d}$	$\mathsf{T}_{12}(0\mathbf{d})$	$p2mm$	$p\underline{2}_y^*m_z\underline{m}_x^*$
		$\frac{1}{4}\mathbf{d}$	$\mathsf{T}_{12}(\frac{1}{4}\mathbf{d})$	$p2_1ma$	$p\underline{2}_{1y}^*m_z\underline{a}_x^*$
		$s\mathbf{d}$	$\mathsf{T}_{12}(s\mathbf{d})$	$p1m1$	$p1m_z1$

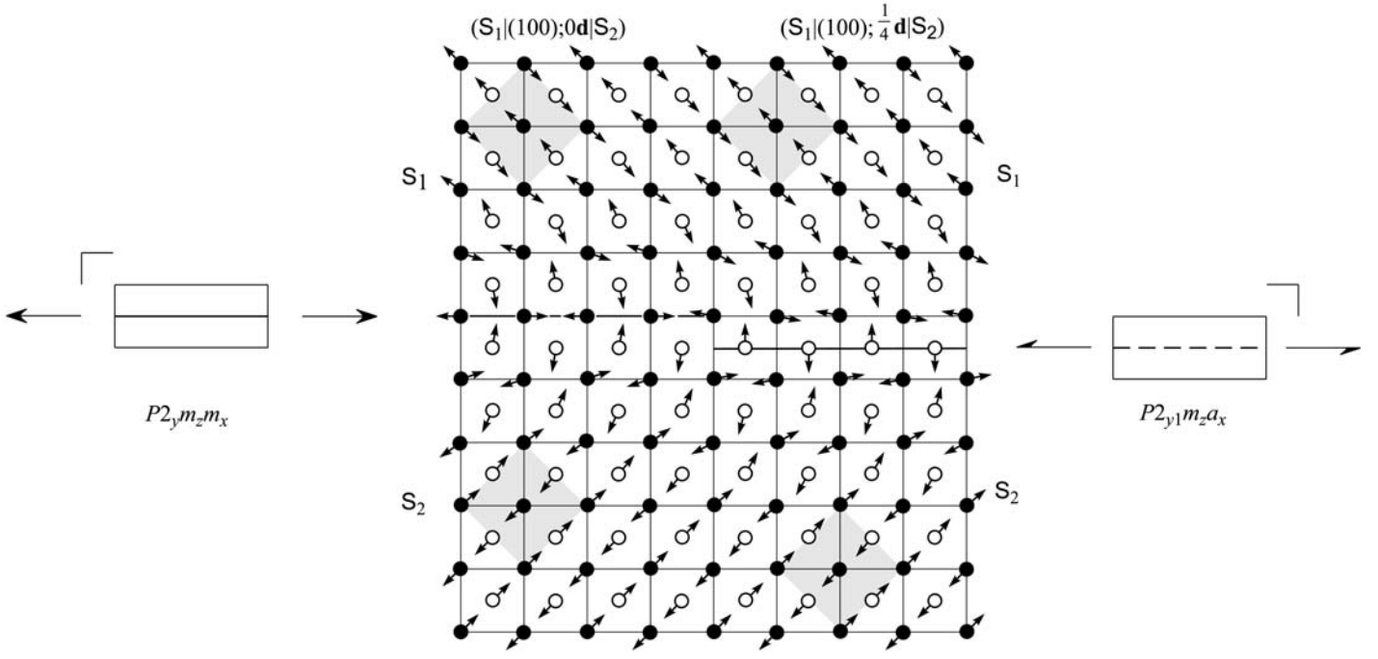

Fig. 5.2.5.7. The structures and symmetries of domain twins in calomel corresponding to two different special positions of the wall.

the figure corresponds to the location of the central plane at $0\mathbf{d}$, the right-hand part to the location at $\frac{1}{4}\mathbf{d}$. The twin symmetries $\mathsf{T}_{12}(0\mathbf{d}) = p2_y m_z m_x$ and $\mathsf{T}_{12}(\frac{1}{4}\mathbf{d}) = p2_{1y} m_z a_x$ determine the relationship between the structures in the two half-spaces. The trivial symmetry operations form the layer group $p1m_z1$ in both cases and leave invariant the structures in both half-spaces. The non-trivial symmetry operations map the structure in one of the half-spaces onto the structure in the other half-space and back. The symmetry of the central plane is given by the groups $\bar{\mathsf{J}}_{12}(0\mathbf{d})$ and $\bar{\mathsf{J}}_{12}(\frac{1}{4}\mathbf{d})$ because the states S_1 and S_2 meet at this plane.

The arrows that represent the shift of calomel molecules in the *xy* plane may rotate and change their amplitude as we approach the central plane because the symmetry requirements are relaxed to those imposed by the layer group $p1m_z1$ consisting of trivial symmetry operations of the twin. The non-trivial twin symmetries determine the relationship between the structures in the two half-spaces, so that the rotation and change of amplitude in these two half-spaces are correlated. The symmetry of the central plane requires, in the left-hand part of the figure, that the arrows at black circles are aligned along the plane and that they are of the same lengths and alternating direction. The arrows at the empty circles in the right-hand part of the figure are nearly perpendicular to the plane, of the same lengths and of alternating direction in accordance with the central-plane symmetry. They are shown in the figure as strictly perpendicular to the plane; however, slight shifts of the atoms parallel to the plane can be expected because the arrows mean that the atoms are actually already out of the central plane.

Summary: In the analysis of domain twins, we know the structures of the two domain states, in our case the orientation of arrows, at infinity. In the example above, we considered two cases in both of which the layer group $\bar{\mathsf{J}}_{12}(s_o\mathbf{d})$ contains all four types of the twin operations – two types of symmetry operations and two types of twin-reversing operations. In this case, we summarize the results of the symmetry analysis as follows. (i) The floating layer group $\widehat{\mathsf{F}}_{12}$ determines the allowed changes of the structures on the path from infinity (physically this means the domain bulk) towards the central plane. (ii) Operations of the coset $t^*_{12}\widehat{F}_{12}$ correlate the changes in the two half-spaces. (iii) The group $\bar{\mathsf{J}}_{12}(s_o\mathbf{d})$ as the symmetry of the central plane where the two half-spaces meet contains the twin symmetry $\mathsf{T}_{12}(s_o\mathbf{d})$ as its halving subgroup and therefore imposes additional conditions on the structure of the central plane in comparison with the conditions in its vicinity.

As always, the symmetry determines only the character of possible changes but neither their magnitude nor their dependence on the distance from the central plane. Thus, in the example considered, the symmetry arguments cannot predict the detailed dependence of the angle of rotation on the distance from the wall and they cannot predict whether and how the lengths of these arrows change.

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