International Tables for Crystallography (2006). Vol. E, Figure 5.2.5.4, p. 412.

(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 $\mathcal{F}_i = g_i\mathcal{F}_1g_i^{-1}$ 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

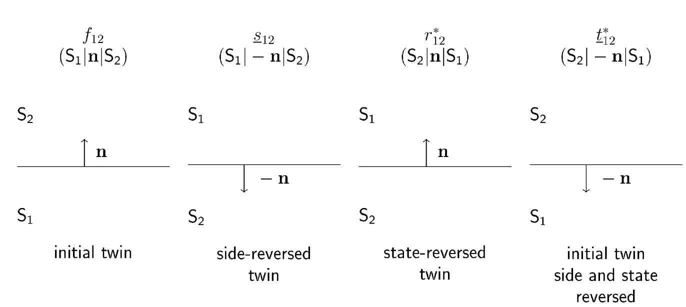

Fig. 5.2.5.4. The four types of operations on a twin.

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