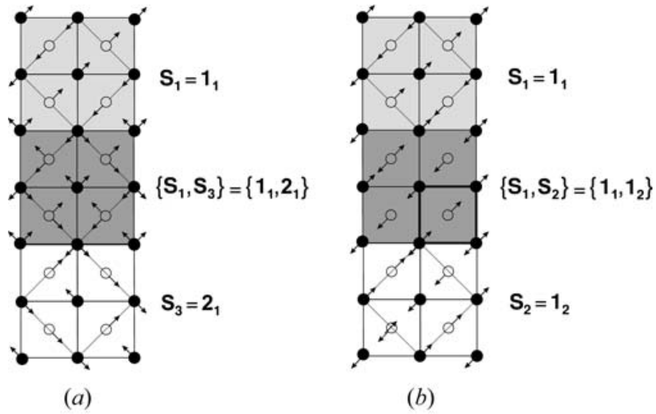

Fig. 3.4.3.10. Domain pairs in calomel. Single-domain states in the parent clamping approximation are those from Fig. 3.4.2.5. The first domain state of a domain pair is shown shaded in grey ('black'), the second domain state is colourless ('white'), and the domain pair of two interpenetrating domain states is shown shaded in dark grey. (*a*) Ferroelastic domain pair $(\mathsf{S}_1, \mathsf{S}_3)$ in the parent clamping approximation. This is a partially transposable domain pair. (*b*) Translational domain pair $(\mathsf{S}_1, \mathsf{S}_2)$. This is a completely transposable domain pair.

Example 3.4.3.8. Ferroelastic crystal of langbeinite. Langbeinite $K_2Mg_2(SO_4)_3$ undergoes a phase transition with symmetry descent $23 \supset 222$ that appears in Table 3.4.3.7. The ferroelastic phase has three ferroelastic domain states. Dudnik & Shuvalov (1989) found, in accord with their theoretical predictions, nearly linear 'almost coherent' domain walls accompanied by elastic stresses in crystals thinner than 0.5 mm. In thicker crystals, elastic stresses became so large that crystals were cracking and no domain walls were observed.

Similar effects were reported by the same authors for the partial ferroelastic phase of $CH_3NH_3Al(SO_4)_2{\cdot}12H_2O$ (MASD) with symmetry descent $\bar{3}m \supset mmm$, where ferroelastic domain walls were detected only in thin samples.

3.4.3.7. *Domain pairs in the microscopic description*

In the *microscopic description*, two microscopic domain states S_i and S_k with space-group symmetries $\mathcal{F}_i$ and $\mathcal{F}_k$, respectively, can form an ordered domain pair $(\mathsf{S}_i, \mathsf{S}_k)$ and an unordered domain pair $\{\mathsf{S}_i, \mathsf{S}_k\}$ in a similar way to in the continuum description, but one additional aspect has to be considered. The definition of the symmetry group $\mathcal{F}_{ik}$ of an ordered domain pair $(\mathsf{S}_i, \mathsf{S}_k)$,

$$\mathcal{F}_{ik} = \mathcal{F}_i \cap \mathcal{F}_k, \qquad (3.4.3.72)$$

is meaningful only if the group $\mathcal{F}_{ik}$ is a space group with a three-dimensional translational subgroup (three-dimensional *twin lattice* in the classical description of twinning, see Section 3.3.8)

$$\mathcal{T}_{ik} = \mathcal{T}_i \cap \mathcal{T}_k, \qquad (3.4.3.73)$$

where $\mathcal{T}_i$ and $\mathcal{T}_k$ are translation subgroups of $\mathcal{F}_i$ and $\mathcal{F}_k$, respectively. This condition is fulfilled if both domain states S_i and S_k have the same spontaneous strains, *i.e.* in non-ferroelastic domain pairs, but in ferroelastic domain pairs one has to suppress spontaneous deformations by applying the parent clamping approximation [see Section 3.4.2.2, equation (3.4.2.49)].

Example 3.4.3.9. Domain pairs in calomel. Calomel undergoes a non-equitranslational phase transition from a tetragonal parent phase to an orthorhombic ferroelastic phase (see Example 3.4.2.7 in Section 3.4.2.5). Four basic microscopic single-domain states are displayed in Fig. 3.4.2.5. From these states, one can form 12 non-trivial ordered single-domain pairs that can be partitioned (by means of double coset decomposition) into two orbits of domain pairs.

Representative domain pairs of these orbits are depicted in Fig. 3.4.3.10, where the first microscopic domain state S_i participating in a domain pair is displayed in the upper cell (light grey) and the second domain state S_j, $j = 2, 3$, in the lower white cell. The overlapping structure in the middle (dark grey) is a geometrical representation of the domain pair $\{\mathsf{S}_1, \mathsf{S}_j\}$.

The domain pair $\{\mathsf{S}_1, \mathsf{S}_3\}$, depicted in Fig. 3.4.3.10(*a*), is a ferroelastic domain pair in the parent clamping approximation. Then two overlapping structures of the domain pair have a common three-dimensional lattice with a common unit cell (the dotted square), which is the same as the unit cells of domain states S_1 and S_3.

Domain pair $\{\mathsf{S}_1, \mathsf{S}_2\}$, shown in Fig. 3.4.3.10(*b*), is a translational (antiphase) domain pair in which domain states S_1 and S_2 differ only in location but not in orientation. The unit cell (heavily outlined small square) of the domain pair $\{\mathsf{S}_1, \mathsf{S}_2\}$ is identical with the unit cell of the tetragonal parent phase (*cf.* Fig. 3.4.2.5).

The two arrows attached to the circles in the domain pairs represent exaggerated displacements within the wall.

Domain pairs represent an intermediate step in analyzing microscopic structures of domain walls, as we shall see in Section 3.4.4.

3.4.4. Domain twins and domain walls

3.4.4.1. *Formal description of simple domain twins and planar domain walls of zero thickness*

In this section, we examine crystallographic properties of planar compatible domain walls and simple domain twins. The symmetry of these objects is described by layer groups. Since this concept is not yet common in crystallography, we briefly explain its meaning in Section 3.4.4.2. The exposition is performed in the continuum description, but most of the results apply with slight generalizations to the microscopic treatment that is illustrated with an example in Section 3.4.4.7.

We shall consider a *simple domain twin* $\mathbf{T}_{12}$ that consists of two domains $\mathbf{D}_1$ and $\mathbf{D}_2$ which meet along a planar domain wall $\mathbf{W}_{12}$ of zero thickness. Let us denote by p a *plane of the domain wall*, in brief *wall plane* of $\mathbf{W}_{12}$. This plane is specified by Miller indices (hkl), or by a normal $\mathbf{n}$ to the plane which also defines the sidedness (plus and minus side) of the plane p. By *orientation of the plane p* we shall understand a specification which can, but may not, include the sidedness of p. If both the orientation and the sidedness are given, then the plane p divides the space into two half-spaces. Using the bra–ket symbols, mentioned in Section 3.4.3.6, we shall denote by $(\,|$ the half-space on the negative side of p and by $|\,)$ the half-space on the positive side of p.

A *simple twin* consists of two (theoretically semi-infinite) domains $\mathbf{D}_1$ and $\mathbf{D}_2$ with domain states $\mathbf{S}_1$ and $\mathbf{S}_2$, respectively, that join along a planar domain wall the orientation of which is specified by the wall plane p with normal $\mathbf{n}$. A symbol $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_2)$ specifies the domain twin unequivocally: domain $(\mathbf{S}_1|$, with domain region $(\,|$ filled with domain state $\mathbf{S}_1$, is on the negative side of p and domain $|\,\mathbf{S}_2)$ is on the positive side of p (see Fig. 3.4.4.1*a*).

If we were to choose the normal of opposite direction, *i.e.* $-\mathbf{n}$, the same twin would have the symbol $(\mathbf{S}_2|-\mathbf{n}|\mathbf{S}_1)$ (see Fig. 3.4.4.1*a*). Since these two symbols signify the same twin, we have the identity

$$(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_2) \equiv (\mathbf{S}_2|-\mathbf{n}|\mathbf{S}_1). \qquad (3.4.4.1)$$

Thus, if we invert the normal $\mathbf{n}$ and simultaneously exchange domain states $\mathbf{S}_1$ and $\mathbf{S}_2$ in the twin symbol, we obtain an identical twin (see Fig. 3.4.4.1*a*). This identity expresses the fact that the