

## 5.2. GUIDE TO THE USE OF THE SCANNING TABLES

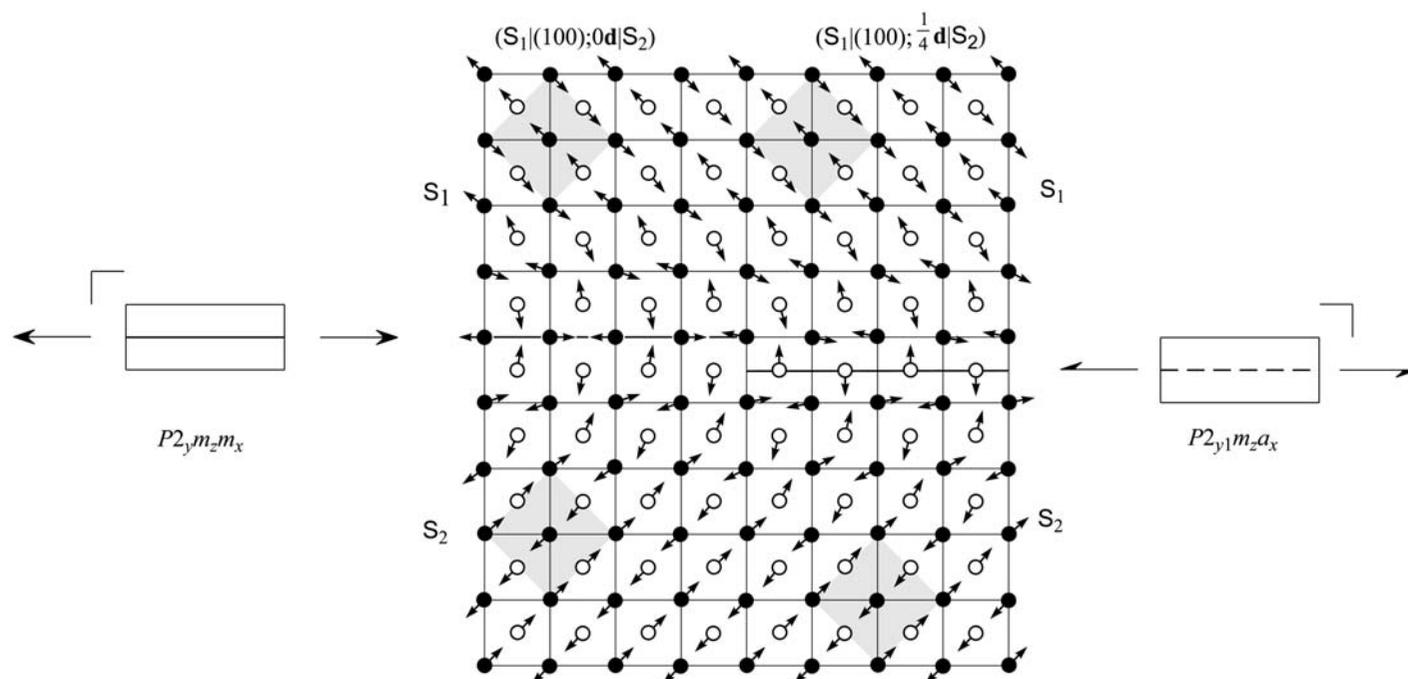


Fig. 5.2.5.7. The structures and symmetries of domain twins in calomel corresponding to two different special positions of the wall.

symmetries  $T_{12}(0\mathbf{d}) = p2_y m_z m_x$  and  $T_{12}(\frac{1}{4}\mathbf{d}) = p2_{y1} m_z a_x$  determine the relationship between the structures in the two half-spaces. The trivial symmetry operations form the layer group  $p1m_z 1$  in both cases and leave invariant the structures in both half-spaces. The nontrivial 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  $\bar{J}_{12}(0\mathbf{d})$  and  $\bar{J}_{12}(\frac{1}{4}\mathbf{d})$  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  $p1m_z 1$  consisting of trivial symmetry operations of the twin. The nontrivial 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  $\bar{J}_{12}(s_o\mathbf{d})$  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  $\hat{F}_{12}$  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  $\hat{L}_{12}^* \hat{F}_{12}$  correlate the changes in the two half-spaces. (iii) The group  $\bar{J}_{12}(s_o\mathbf{d})$  as the symmetry of the central plane where the two half-spaces meet contains the twin symmetry  $T_{12}(s_o\mathbf{d})$  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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## 5. SCANNING OF SPACE GROUPS

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