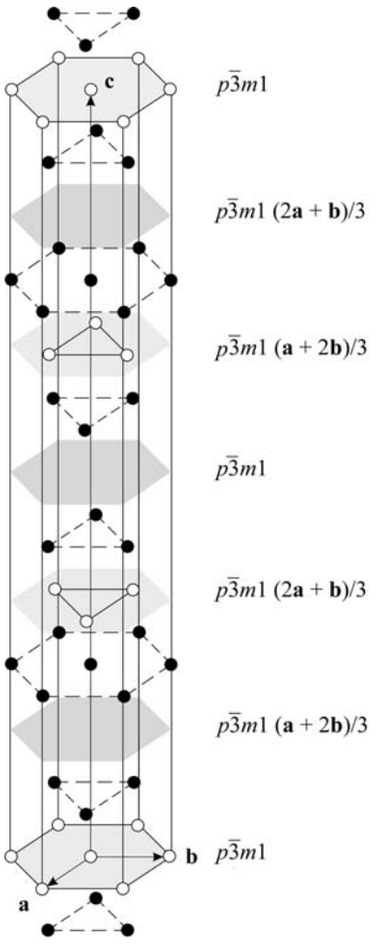

Fig. 5.2.5.2. The structure of cadmium chloride, CdI_2. The section planes of two orbits in special positions are distinguished by shading. Notice the different location of the sectional layer groups on different levels for the same orbit. The figure is drastically elongated in the *c* direction to exhibit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

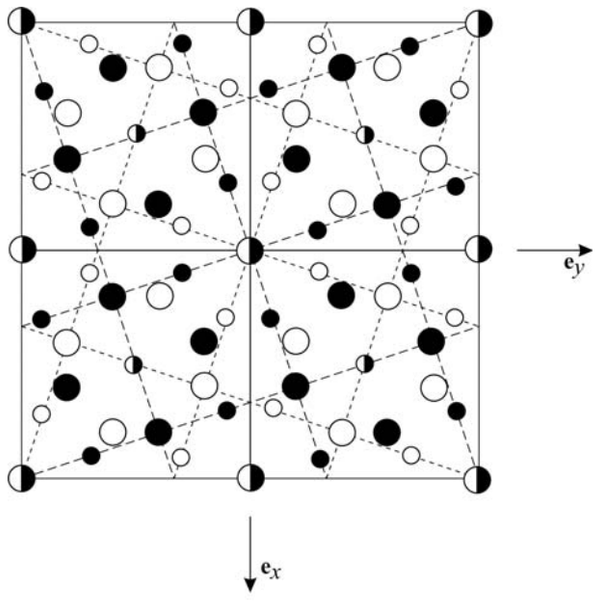

Fig. 5.2.5.3. A classical example of a bicrystal (Vlachavas, 1985).

references