$P\bar{6}m2$, $P6_3mc$, $P6_3/mmc$, $R3m$, $R\bar{3}m$, and $Fm3m$. The last space group corresponds to the special case of cubic close packing $/ABC/\ldots$. The tetrahedral arrangement of Si and C in SiC does not permit either a centre of symmetry ($\bar{1}$) or a plane of symmetry (m) perpendicular to [00.1]. SiC structures can therefore have only four possible space groups $P3m1$, $R3m1$, $P6_3mc$, and $F\bar{4}3m$. CdI_2 structures can have a centre of symmetry on octahedral voids, but cannot have a symmetry plane perpendicular to [00.1]. CdI_2 can therefore have five possible space groups: $P3m1$, $P\bar{3}m$, $R3m$, $R\bar{3}m$, and $P6_3mc$. Cubic symmetry is not possible in CdI_2 on account of the presence of Cd atoms, the sequence $/A\gamma BC\beta AB\alpha C/$ representing a 6R structure.

9.2.1.6. *Crystallographic uses of Zhdanov symbols*

From the Zhdanov symbols of a close-packed structure, it is possible to derive information about the symmetry and lattice type (Verma & Krishna, 1966). Let n_+ and n_- be the number of positive and negative numerals in the Zhdanov sequence of a given structure. The lattice is rhombohedral if $n_+ - n_- = \pm 1 \bmod 3$, otherwise it is hexagonal. The + sign corresponds to the reverse setting and − to the obverse setting of the rhombohedral lattice. Since this criterion is sufficient for the identification of a rhombohedral structure, the practice of writing three units of identical Zhdanov symbols has been abandoned in recent years (Pandey & Krishna, 1982*a*). Thus the 15R polytype of SiC is written as (23) rather than $(23)_3$.

As described in detail by Verma & Krishna (1966), if the Zhdanov symbol consists of an odd set of numbers repeated twice, *e.g.* (22), (33), (221221) *etc.*, the structure can be shown to possess a 6_3 axis. For the centre of symmetry at the centre of a sphere or an octahedral void, the Zhdanov symbol will consist of a symmetrical arrangement of numbers of like signs surrounding a single even or odd Zhdanov number, respectively. Thus, the structures (2)32(4)23 and (3)32(5)23 have centres of symmetry of the two types in the numbers within parentheses. For structures with a symmetry plane perpendicular to [00.1], the Zhdanov symbols consist of a symmetrical arrangement of a set of numbers of opposite signs about the space between two succession numbers. Thus, a stacking |522|225| has mirror planes at positions indicated by the vertical lines.

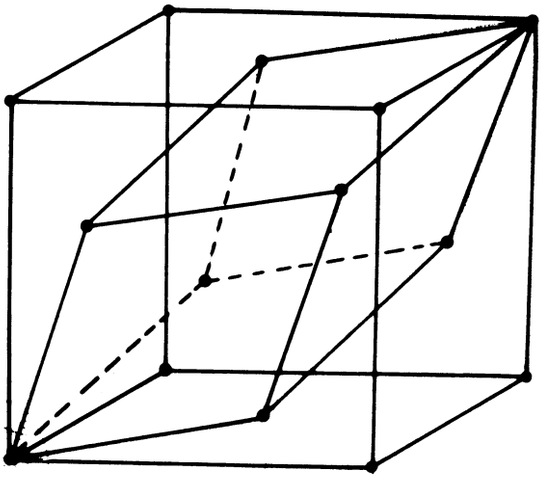

Fig. 9.2.1.8. The relationship between the f.c.c. and the primitive rhombohedral unit cell of the c.c.p. structure.

The use of abridged symbols to describe crystal structures has sometimes led to confusion in deciding the crystallographic equivalence of two polytype structures. For example, the structures (13) and (31) are identical for SiC but not for CdI_2 (Jain & Trigunayat, 1977*a*,*b*).

9.2.1.7. *Structure determination of close-packed layer stackings*

9.2.1.7.1. *General considerations*

The different layer stackings (polytypes) of the same material have identical a and b parameters of the direct lattice. The a^*b^* reciprocal-lattice net is therefore also the same and is shown in Fig. 9.2.1.9. The reciprocal lattices of these polytypes differ only along the c^* axis, which is perpendicular to the layers. It is evident from Fig. 9.2.1.9 that for each reciprocal-lattice row parallel to $\mathbf{c}^*$ there are five others with the same value of the radial coordinate ξ. For example, the rows 10.l, 01.l, $\bar{1}1.l$, $\bar{1}0.l$, $0\bar{1}.l$, and $1\bar{1}.l$ all have $\xi = |\mathbf{a}^*|$. Owing to symmetry considerations, it is sufficient to record any one of them on X-ray diffraction photographs. The reciprocal-lattice rows $hk.l$ can be classified into two categories according as $h - k = 0 \bmod 3$ or $\pm 1 \bmod 3$. Since the atoms in an nH or nR structure lie on three symmetry axes $A : [00.1]_{00}$, $B : [00.1]_{\frac{1}{3},-\frac{1}{3}}$, and $C : [00.1]_{-\frac{1}{3},\frac{1}{3}}$, the structure factor F_{hkl} can be split into three parts:

$$F_{hkl} = P + Q\exp[2\pi i(h-k)/3] + R\exp[-2\pi i(h-k)/3],$$

where $P = \sum_{z_A} \exp(2\pi i l z_A/n)$, $Q = \sum_{z_B} \exp(2\pi i l z_B/n)$, $R = \sum_{z_C} \exp(2\pi i l z_C/n)$, and z_A/n, z_B/n, z_C/n are the z coordinates of atoms at A, B, and C sites, respectively. For $h - k = 0 \bmod 3$,

$$F_{hkl} = P + Q + R = \sum_{z=0}^{n=-1} \exp(2\pi i l z/n),$$

which is zero except when $l = 0, n, 2n, \ldots$. Hence, the reflections 00.l, 11.l, 30.l, *etc.*, for which $h - k = 0 \bmod 3$, will be extinguished except when $l = 0, n, 2n, \ldots$. Thus, only those $hk.l$ reciprocal-lattice rows for which $h - k \neq 0 \bmod 3$ carry information about the stacking sequence and contain in general reflections with $l = 0, 1, 2, \ldots, n-1$, *etc.* It is sufficient to record any one such row, usually the 10.l row with $\xi = |\mathbf{a}^*|$, on an oscillation, Weissenberg, or precession photograph to obtain information about the lattice type, identity period, space group, and hence the complete structure (Verma & Krishna, 1966).

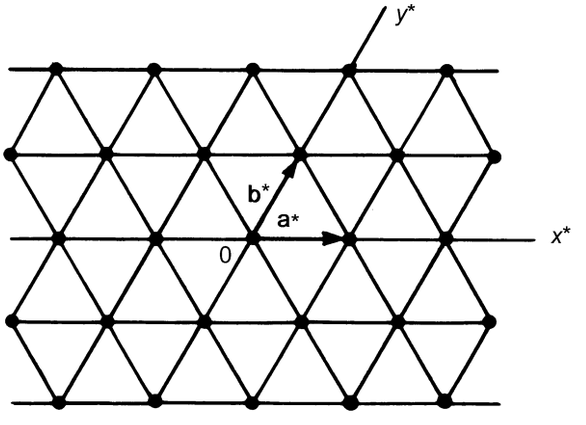

Fig. 9.2.1.9. The $\mathbf{a}^*$–$\mathbf{b}^*$ reciprocal-lattice net for close-packed layer stackings.

references