Face Centered Cubic Lattice

No of electrons per primitive unit cell

(In cubic non-prim cell (1,1,1)
4x4 from 1/2 shifted site
+ 1/8 from corner site bonds in cell
+ 3x6/2 shaded = 3.2 \rightarrow 8 primitive cells/unit cell \rightarrow 8 electrons per primitive cell

Note on Ga-As

\( \bar{a} = \frac{a}{2} (\bar{x} + \bar{y}) \)

\( \bar{b} = \frac{a}{2} (\bar{x} + \bar{z}) \)

\( \bar{c} = \frac{a}{2} (\bar{z} + \bar{y}) \)

\( \frac{2\pi a^2}{a^2} \frac{(-\frac{1}{2} + \frac{1}{3} - \frac{1}{2})}{(a/8)} \)

\( \frac{2\pi}{a} (\bar{x}, \bar{y}, \bar{z}) \)

\( m \bar{a} + n \bar{b} + p \bar{c} = \frac{2\pi a}{a} (\bar{x}, \bar{y}, \bar{z}) \)

to get \( \bar{x} = n = 0 \) \( m = p \) lattice vector = \( \frac{2\pi a}{a} \)

\( m = n = p = 1 \) \( \frac{2\pi a}{a} (\bar{x}, \bar{y}, \bar{z}) \)

Length = \( 2\pi a \frac{\sqrt{3}}{2} \) \( \rightarrow \) Brillouin \( \frac{2\pi}{a} \)

\( E = \frac{h^2}{2m} (k_x - \frac{2\pi}{a} (-m+n-p))^2 + (k_y - \frac{2\pi}{a} (m-n-p))^2 + (k_z - \frac{2\pi}{a} (-m+n+p))^2 \)
From Wooten Optical Properties of Solids

1.1 Band Theory of Solids

The band theory of solids is based on a one-electron approximation. That is, an electron is assumed to be acted on by the field of the fixed atomic cores plus an average field arising from the charge distribution of all the other outer-shell electrons. The atomic cores consist of the nuclei and all inner-shell electrons not appreciably perturbed by neighboring atoms. If the solid is a perfect crystal, the total crystal potential energy \( V(r) \) must have the periodicity of the crystal lattice. On the basis of this model, the solutions of the Schrödinger equation

\[
(h^2/2m) \nabla^2 \psi + [\mathbf{\varepsilon} - V(r)] \psi = 0 \tag{1.1}
\]

are Bloch functions

\[
\psi(k, r) = u_k(r) \exp(ik \cdot r) \tag{1.2}
\]

where \( u_k(r) \) is a function having the periodicity of the lattice.

The simplest solution to Eq. (1.1) is for the case in which \( V(r) \) is constant and can be taken as zero. It leads to free electrons and plane waves for wave functions. The energy of an electron is then given by

\[
\mathbf{\varepsilon} = h^2 k^2 / 2m \tag{1.3}
\]

If we include the periodicity of the lattice, but say that the perturbing potential is arbitrarily weak, the energy of an electron can be expressed as

\[
\mathbf{\varepsilon} = (h^2/2m) |k + \mathbf{G}|^2 \tag{1.4}
\]

where \( \mathbf{G} \) is a reciprocal lattice vector. The energy bands are then best represented in the reduced zone scheme. Figure 1.1 shows the free-electron

Fig. 1.1 Free-electron energy band structure in the reduced zone scheme for face-centered-cubic lattices. The Fermi level is shown for different numbers of outer shell electrons per unit cell. The degeneracy (other than the twofold spin degeneracy) of each energy band segment is indicated by the number of dots on the corresponding line. Symmetry points in the reduced zone (inset) are identified by Greek or Roman letters. The lattice constant (unit cell edge) is denoted by \( a \). This diagram applies to such crystals as Al, Cu, Ag, Ge, and GaAs: it includes most of the solids discussed in detail in the book. [From F. Herman, Atomic Structure, in "An Atomistic Approach to the Nature and Properties of Materials" (J. A. Park, ed.). Wiley, New York, 1967.]