2 Energy Bands in Crystals

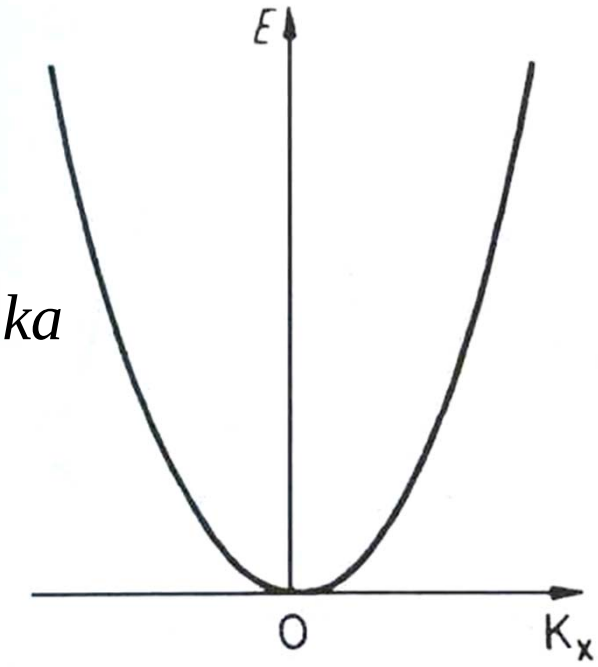
2.1 One-Dimensional Zone Schemes

*** For Free electron**

$$E = \frac{\hbar^2}{2m} k_x^{\,2} \quad \Rightarrow \quad k_x = \text{const} \cdot E^{1/2}.$$

$$P\frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka \quad \Rightarrow \quad \cos \alpha a = \cos ka$$

since P=0



$$\cos \alpha a = \cos k_x a = \cos(k_x a + n2\pi),$$

$$\alpha a = k_x a + n2\pi.$$

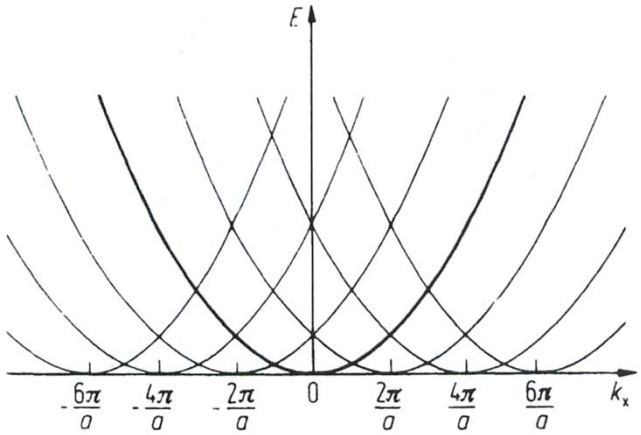
$$\alpha = \sqrt{\frac{2m}{\hbar^2}} E^{1/2}, \quad k_x + n\frac{2\pi}{a} = \sqrt{\frac{2m}{\hbar^2}} E^{1/2}.$$

We see that in the general case the parabola, above is repeated periodically in intervals of n·2π/a.

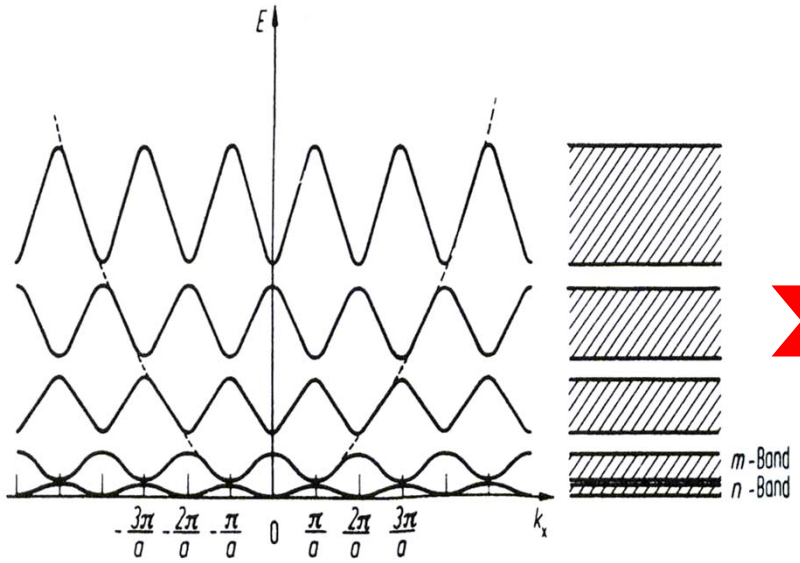
If an electron propagates in a periodic potential we always observe discontinuities of the energies when $\cos k_x a$ has a maximum or a minimum, i.e., when $\cos k_x a = \pm 1$

$$k_x a = n\pi, \quad n = \pm 1, \ \pm 2, \ \pm 3, \ \ldots,$$

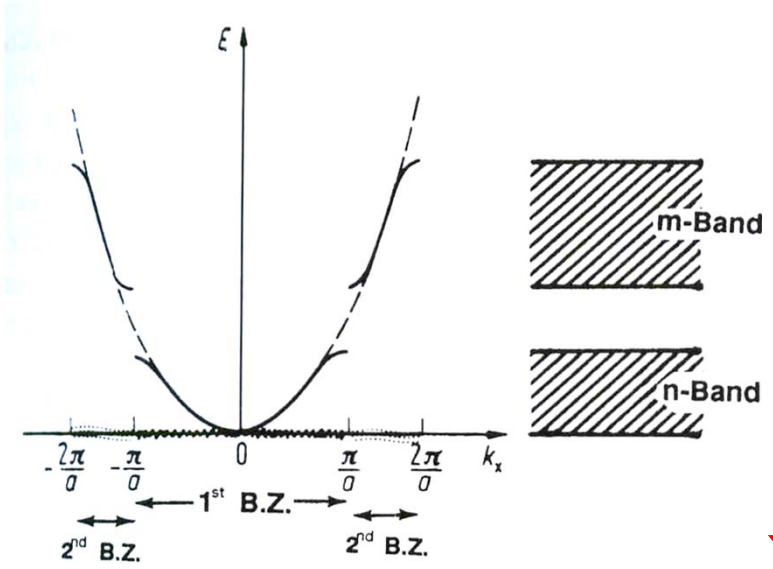
$$k_x = \frac{n\pi}{a}$$



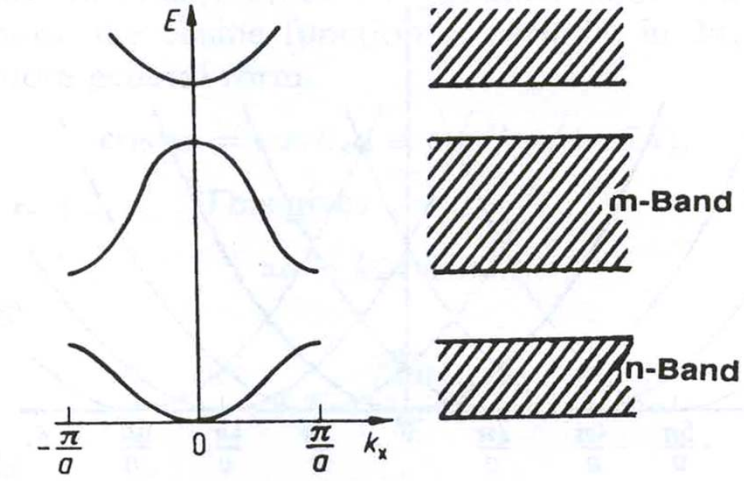
At these singularities, a deviation from the parabolic E versus k_x curve occurs and the branches of the individual parabola merge into the neighboring ones.



The electrons in a crystal behave, for most k_x values, like free electrons, except when k_x approaches the value $n\pi/a$.



"Extended zone scheme"



"Reduced zone scheme"

We call the allowed bands,for the time being, the n-band,or the m-band, and so forth. In later sections and particularly in semiconductor physics we will call one of these bands the **valence band** and the next higher one the **conduction band**

Plotting free electrons in a reduced zone scheme:

width of the forbidden bands to be reduced until the energy gab disappears completely.

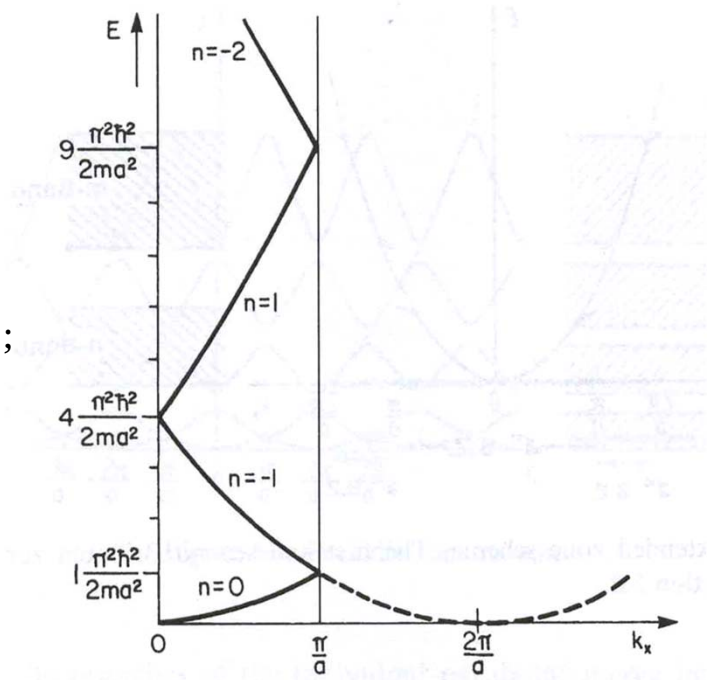
$$E = \frac{\hbar^2}{2m}\left(k_x + n\frac{2\pi}{a}\right)^2, \qquad n = 0,\ \pm 1,\ \pm 2,\ ....$$

$\mathrm{n} = 0$ yields $E = \frac{\hbar^2}{2m}k_x^2$ (parabola with 0 as origin);

$\mathrm{n} = -1$ yields $E = \frac{h^2}{2m}\left(k_x - \frac{2\pi}{a}\right)^2$ $\left(\text{parabola with } \frac{2\pi}{a} \text{ as origin}\right)$;

specifically, for k_x=0 follows $E = 4\frac{\pi^2\hbar^2}{2ma^2}$;

and for $k_x = \frac{\pi}{\mathrm{a}}$ follows $E = 1\frac{\pi^2\hbar^2}{2ma^2}$.



Free electron bands

The energy versus k_x curve, between -π/a and π/a, corresponds to the first electron band -- this region in k-space is called the first Brillouin zone (BZ).
Accordingly, the area between π/a and 2π/a, and also between -π/a and -2π/a is called the second BZ.
-- We do not need to plot E versus k curves for all BZ; the relevant information is, because of the 2π/a periodicity, already contained in the first BZ.

2.2 One-and Two-Dimensional Brillouin Zones

The electron movement in 2-D can be described by the wave vector **k** that has component k_x and k_y which are parallel to the x-axis and y-axis in reciprocal space.

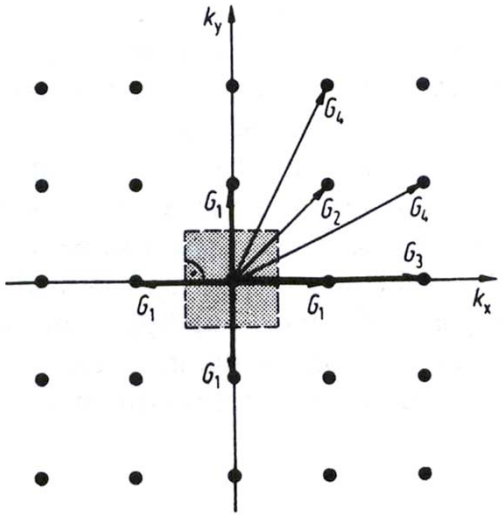
Points in the k_x-k_y coordinate system form a 2-D reciprocal lattice.

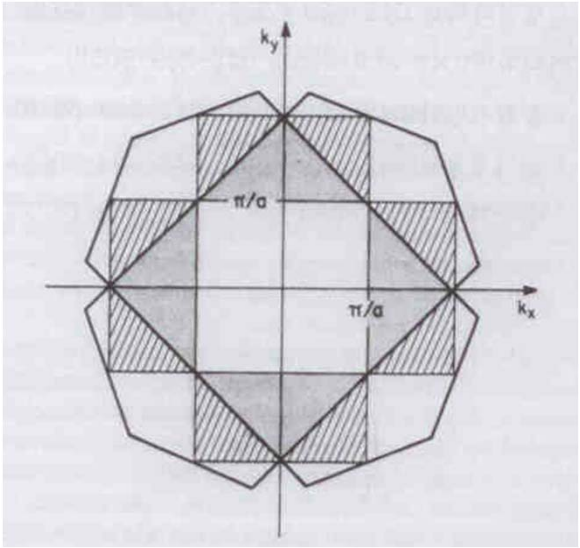
Construction of the BZ for 2-D reciprocal space:

For the first BZ – one constructs the perpendicuar bisectors on the shortest lattice vectors, G_1
The area that is enclosed by these four "Bragg planes" is the first BZ

For the following zones the bisectors of the next shortest lattice vectors are constructed.
.....

Note that all the zones have the same area.





2.2 One-and Two-Dimensional Brillouin Zones

The BZs are useful if one wants to calculate the behavior of an electron which may travel in a specific direction in reciprocal space.

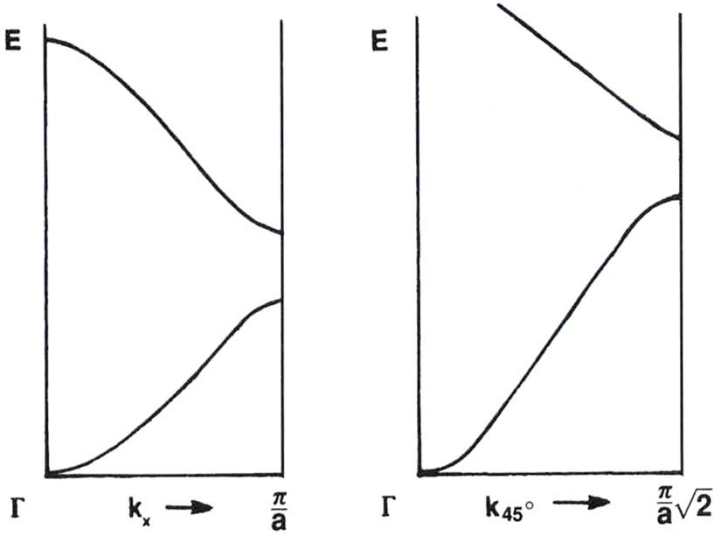
For an electron travels at 45° to the kx-axis, then the boundary of the BZ is reached for,

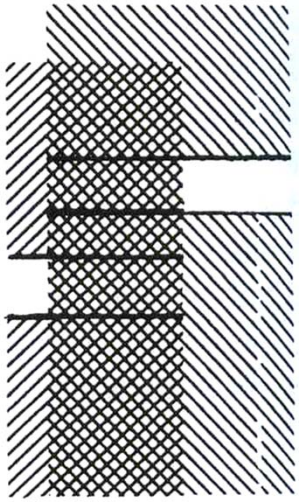
$$k_{crit} = \frac{\pi}{a}\sqrt{2} \quad E_{\max} = \frac{\hbar^2 k_{crit}^2}{2m} = \frac{\pi^2 \hbar^2}{a^2 m}$$

For an electron travels parallel to the kx- or ky-axes,

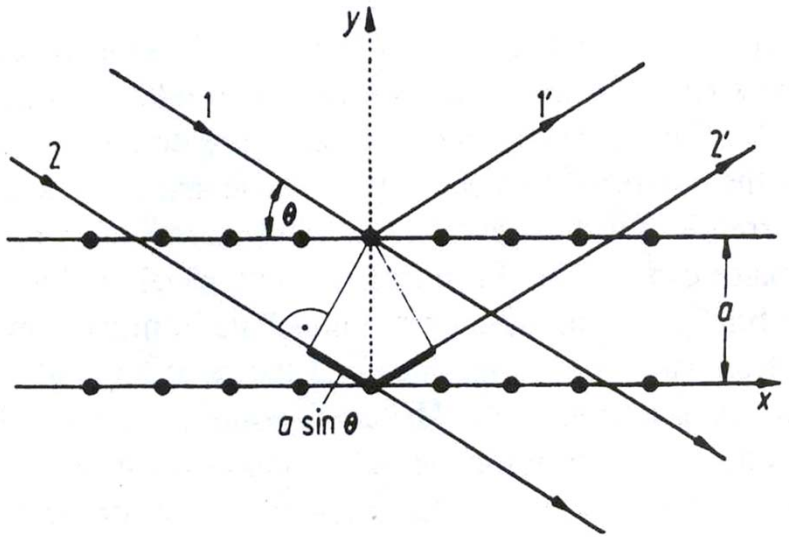
$$k_{crit} = \frac{\pi}{a} \quad E_{\max} = \frac{1}{2}\left(\frac{\pi^2 \hbar^2}{a^2 m}\right)$$

Once the maximum energy is reached, the electron waves form standing waves – electrons reflected back into the BZ.





In previous pages we have seen an electron **traveling in a specific direction** , When we consider energies with all direction, **overlapping of allowed energy bands** occur



(Bragg Reflection)

$$2a\sin\theta = n\lambda, \qquad n = 1, 2, 3, \ldots$$

$$2a\sin\theta = n\frac{2\pi}{k}$$

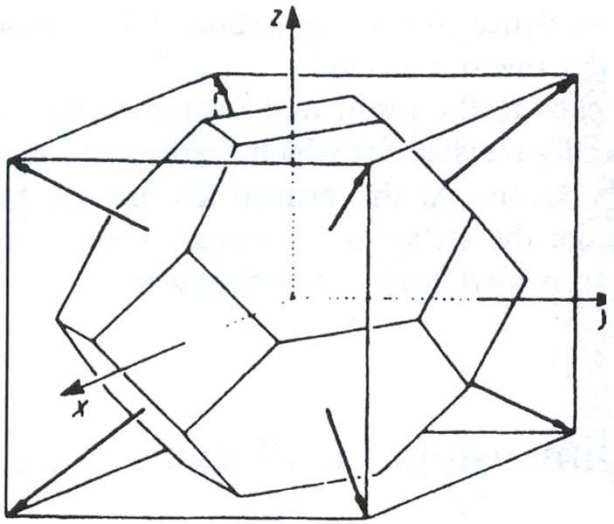
$$\boxed{k_{\text{crit}} = n\frac{\pi}{a\sin\theta}.}$$

2.3 3-D Brillouin Zone and Wigner-Seitz Cells

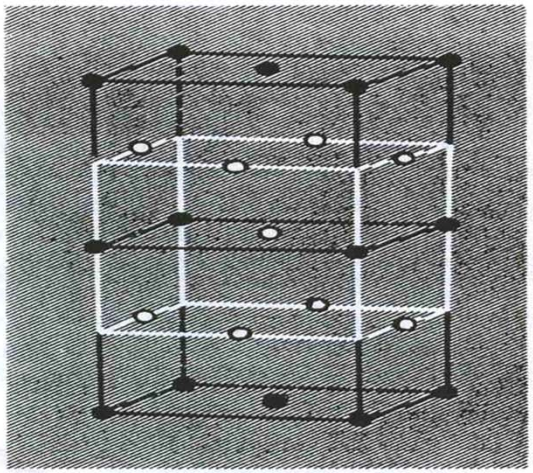
Crystals have symmetrical properties. Therefore, a crystal can be described as an accumulation of **"unit cells".** There are two kinds of unit cell, **"primitive unit cell"** means a smallest possible cell, and **"conventional unit cell"** is a nonprimitive unit cell having the advantage that the symmetry can be better recognized,

➡ **Wigner-Seitz Cell is a special type of primitive unit cell that shows the cubic symmetry of the cubic cells.**

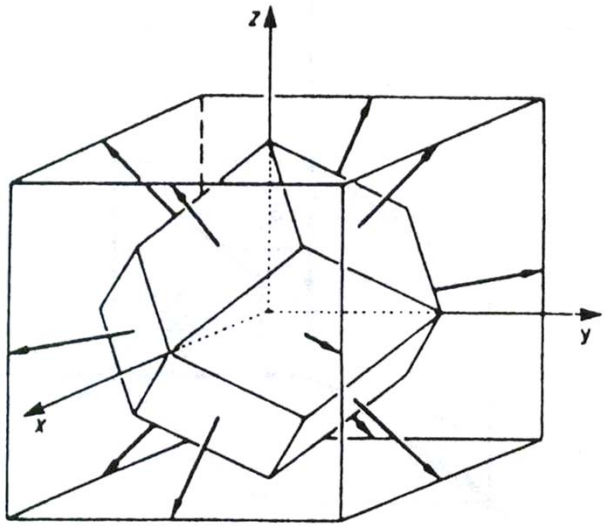
One bisects the vectors from a given atom to its nearest neighbors and places a plane perpendicular to these vectors at the bisecting points.



Wigner-Seitz cell (BCC)



Conventional unit cell (FCC)



Wigner-Seitz cell (FCC)

2.4 Translation Vectors and the Reciprocal Lattice

$$\mathbf{R} = n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3,$$

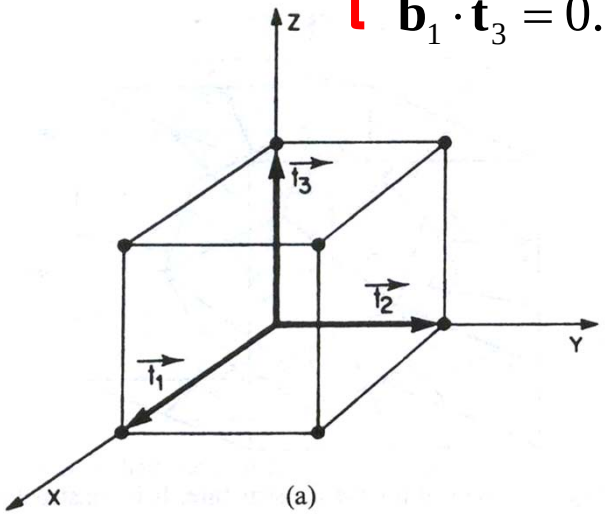
Primitive vectors or translation vector

$$\mathbf{G} = 2\pi(h_1\mathbf{b}_1 + h_2\mathbf{b}_2 + h_3\mathbf{b}_3),$$

$\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$: *reciprocal lattice vectors*

$$\begin{aligned} \mathbf{b}_1 \cdot \mathbf{t}_1 &= 1, \\ \mathbf{b}_1 \cdot \mathbf{t}_2 &= 0, \\ \mathbf{b}_1 \cdot \mathbf{t}_3 &= 0. \end{aligned}$$

$$\mathbf{b}_n \bullet t_m = \delta_{mn}$$



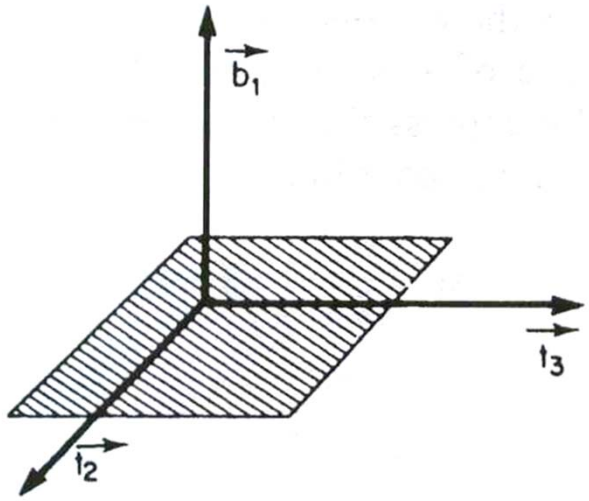


Fig. 5.15

$$\mathbf{b}_1 = \text{const.}\,\mathbf{t}_2 \times \mathbf{t}_3.$$

$$\mathbf{b}_1 \cdot \mathbf{t}_1 = \text{const.}\,\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3 = 1.$$

$$\text{const.} = \frac{1}{\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3}.$$

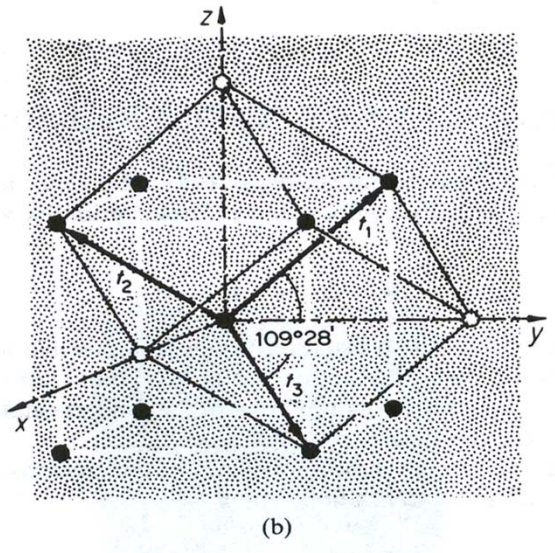
$$\therefore \mathbf{b}_1 = \frac{\mathbf{t}_2 \times \mathbf{t}_3}{\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3}.$$

$$\mathbf{b}_2 = \frac{\mathbf{t}_3 \times \mathbf{t}_1}{\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3}, \quad \mathbf{b}_3 = \frac{\mathbf{t}_1 \times \mathbf{t}_2}{\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3}.$$

For BCC,

$$\mathbf{t}_1 = \frac{a}{2}(-\mathbf{i} + \mathbf{j} + \mathbf{k}),$$

$$\mathbf{t}_1 = \frac{a}{2}(\bar{1}11) \quad \mathbf{t}_2 = \frac{a}{2}(1\bar{1}1), \quad \mathbf{t}_3 = \frac{a}{2}(11\bar{1}).$$



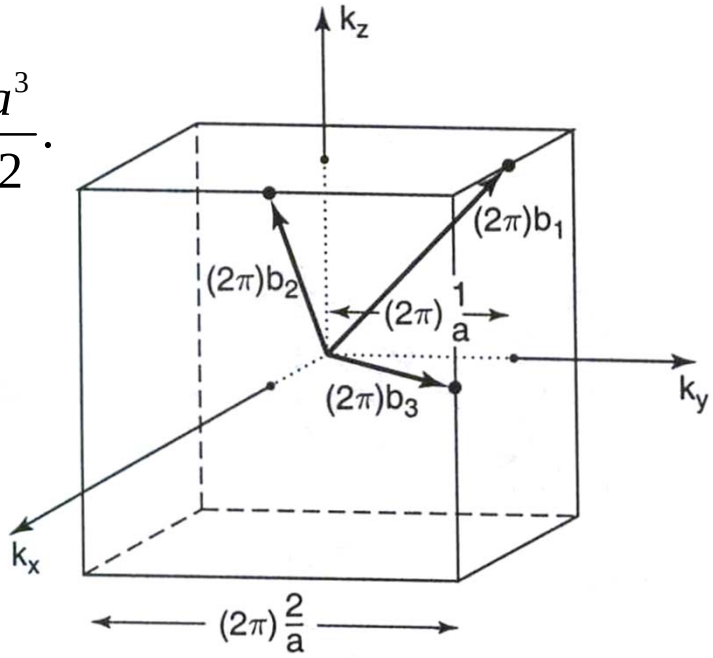
$$\mathbf{t}_2 \times \mathbf{t}_3 = \frac{a^2}{4}\begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix} = \frac{a^2}{4}(2\mathbf{j}+2\mathbf{k})$$

$$= \frac{a^2}{2}(\mathbf{j}+\mathbf{k})$$

$$\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3 = \frac{a^3}{4}(-\mathbf{i}+\mathbf{j}+\mathbf{k})\cdot(0+\mathbf{j}+\mathbf{k}) = \frac{a^3}{4}(0+1+1) = \frac{a^3}{2}.$$

$$\mathbf{b}_1 = \frac{\frac{a^2}{2}(\mathbf{j}+\mathbf{k})}{\frac{a^3}{2}} = \frac{1}{a}(\mathbf{j}+\mathbf{k}),$$

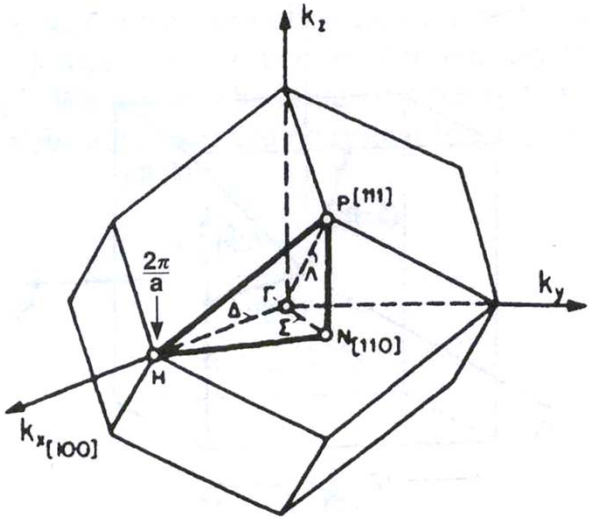
$$\mathbf{b}_1 = \frac{1}{a}(011). \quad \mathbf{b}_2 = \frac{1}{a}(101). \quad \mathbf{b}_3 = \frac{1}{a}(110).$$



The end points of the reciprocal lattice vectors of a bcc crystal are at the center of the edges of a cube. This means that reciprocal lattice of the bcc structure are identical to the lattice points in a real lattice of the fcc structure

Brillouin zone can be defined as a Wigner-Seitz cell in the reciprocal length.

2.5 Free Electron Bands



$\Gamma : (000)$ origin

$\Gamma \to H_{[100]} : \Delta, \quad \Gamma \to N_{[110]} : \Sigma, \quad \Gamma \to P_{[111]} : \Lambda$

select $\Gamma \to H$ as an example,

$$\mathbf{k}' = \mathbf{k} + \mathbf{G}.$$

$$E_{k'} = \frac{\hbar^2}{2m}(\mathbf{k}+\mathbf{G})^2. \quad E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}x\mathbf{i}+\mathbf{G}\right)^2,$$

$$E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 (x\mathbf{i})^2 \equiv Cx^2, C = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 = \frac{2\hbar^2\pi^2}{ma^2}$$

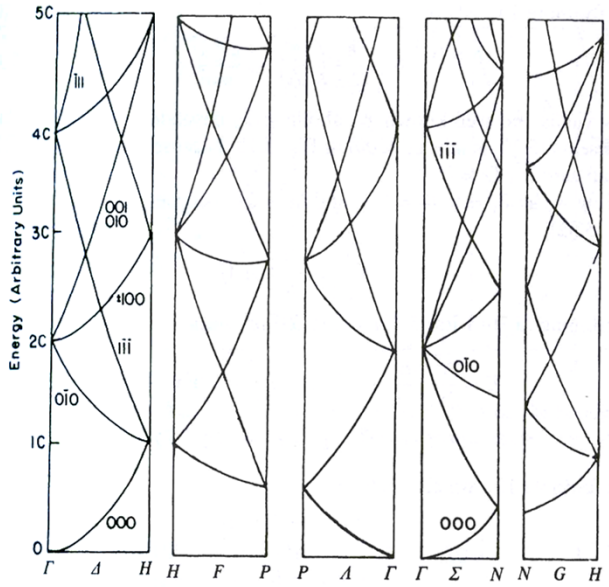
$$\mathbf{G} = -\frac{2\pi}{a}(\mathbf{i}+\mathbf{l}).$$

$$E = \frac{h^2}{2m}\left[\frac{2\pi x}{a}\mathbf{i} - \frac{2\pi}{a}(\mathbf{i}+\mathbf{l})\right]^2 = C\left[\mathbf{i}(x-1)-\mathbf{l}\right]^2$$

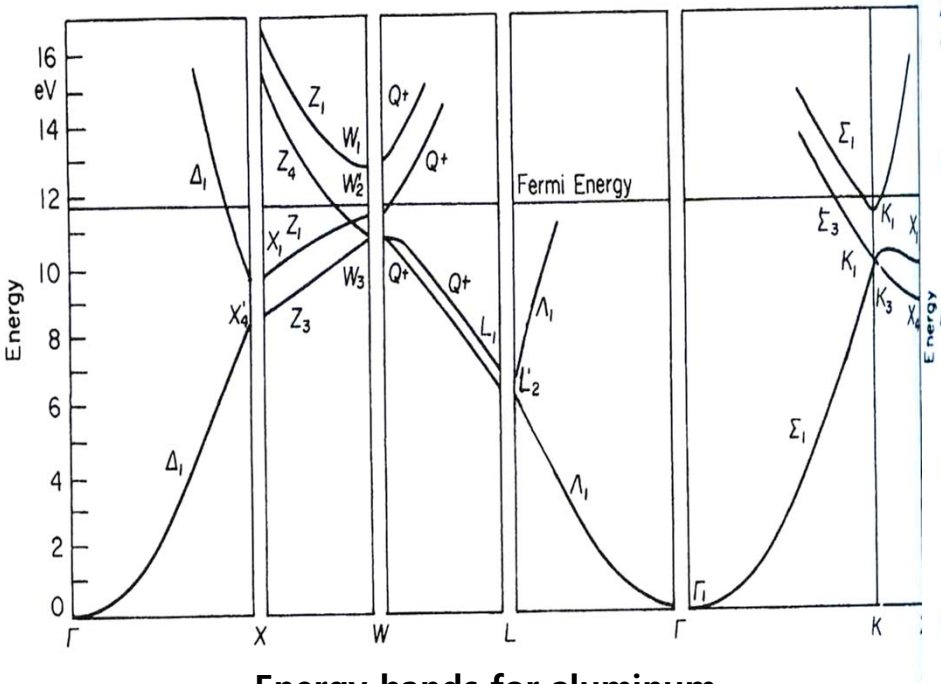
$$= C\left[(x-1)^2+1\right] = C\left(x^2-2x+2\right)$$

$x = 0 \to E = 2C$

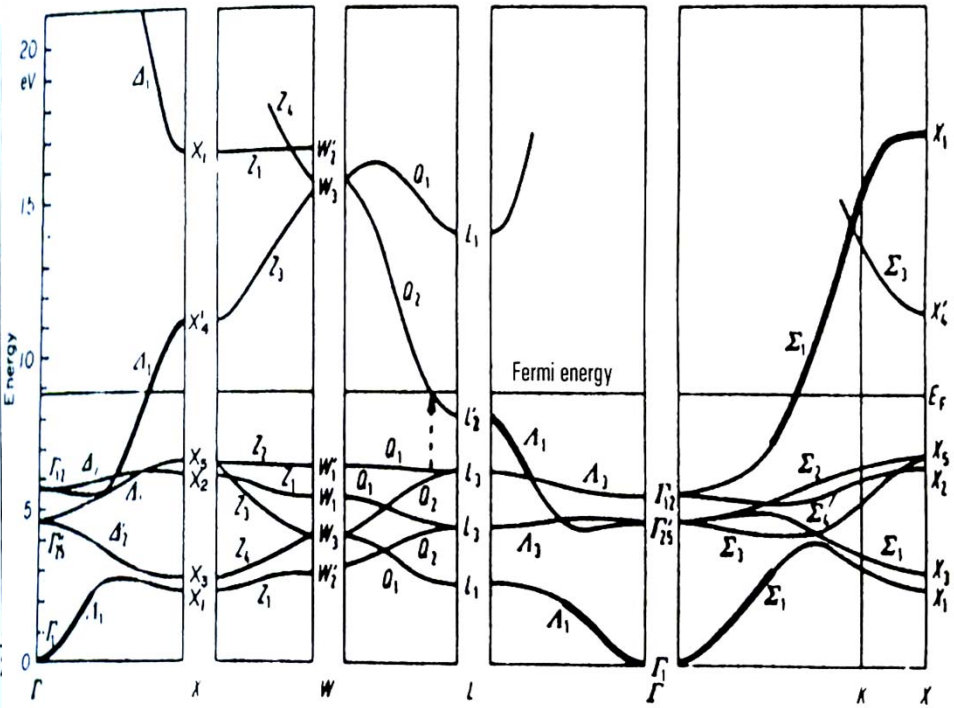
$x = 1 \to E = 1C.$



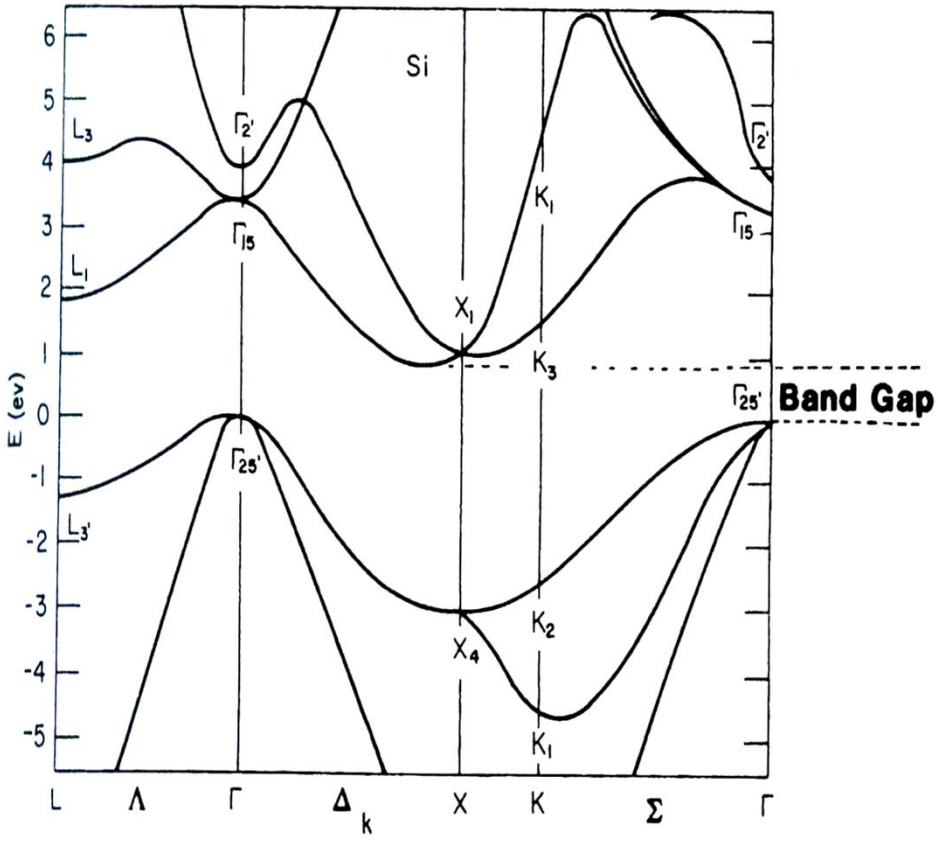
2.6 Band Structures for Some Metals and Semiconductors



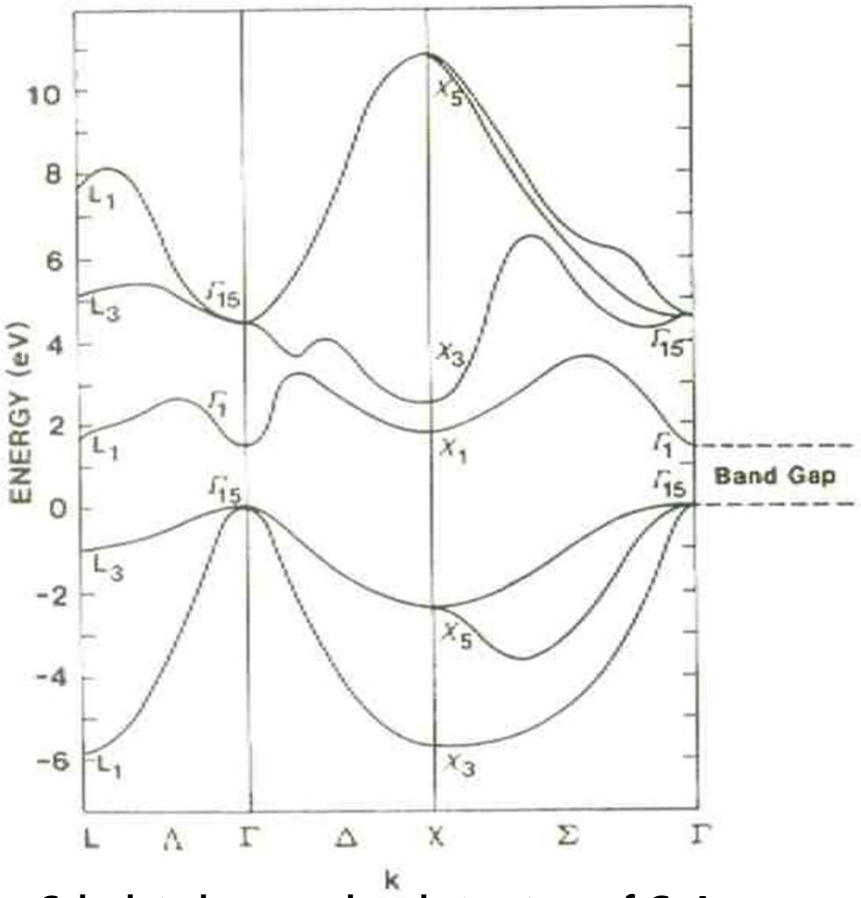
Energy bands for aluminum



Band structure of copper (fcc)



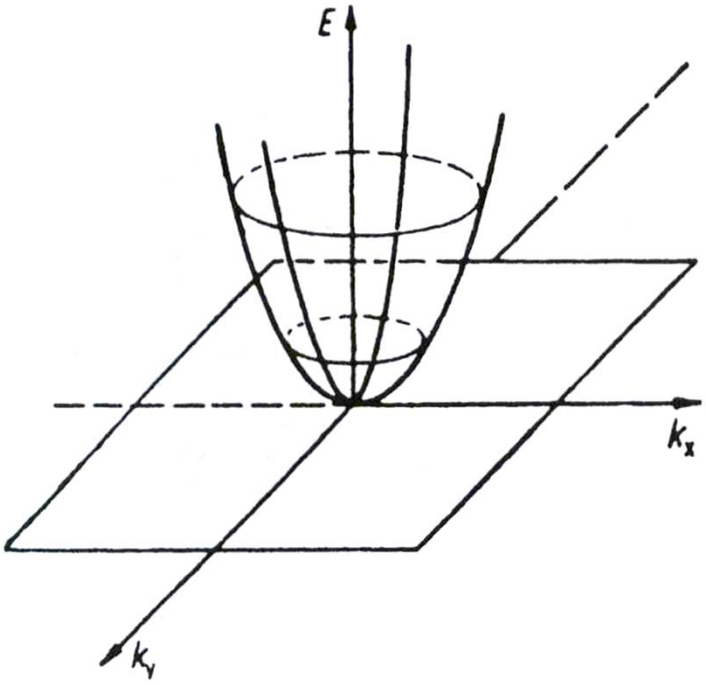
Calculated energy band structure of silicon (diamond-cubic crystal)



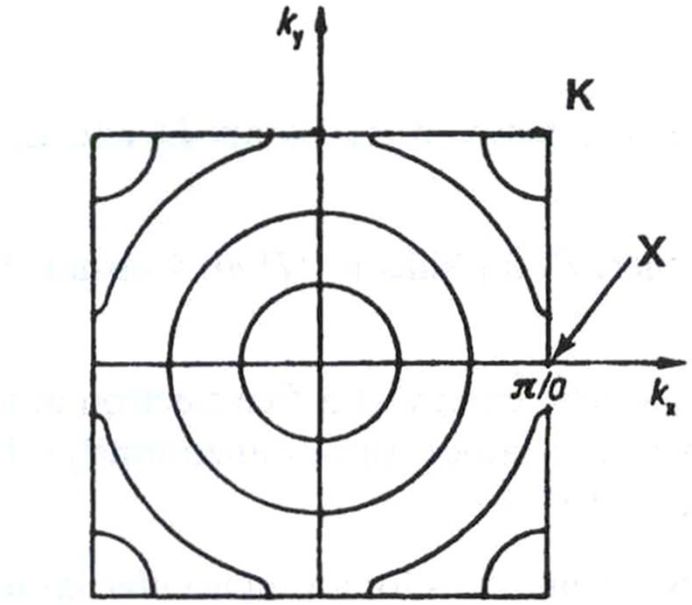
Calculated energy band structure of GaAs.

2.7 Curves and Planes of Equal Energy

In 1-D **k**-space, there is only one positive **k**-value which is connected with a given energy. In 2-D, when we plot the electron energy over a k_x-k_y plane, more than one **k**-value can be assigned to a given energy – leads to curves of equal energy.



Electron energy E versus wave vector



Curves of equal energy inserted into the first Brillouin zone for 2-D square lattice