Effective Mass

The electrons in energy bands, behave differently to that of free-electrons (in a vacuum). This means the electron in a crystal is not completely free, but its acceleration in a crystal a is influenced by both external and internal forces, see Figure 13, E_x is the electric field:

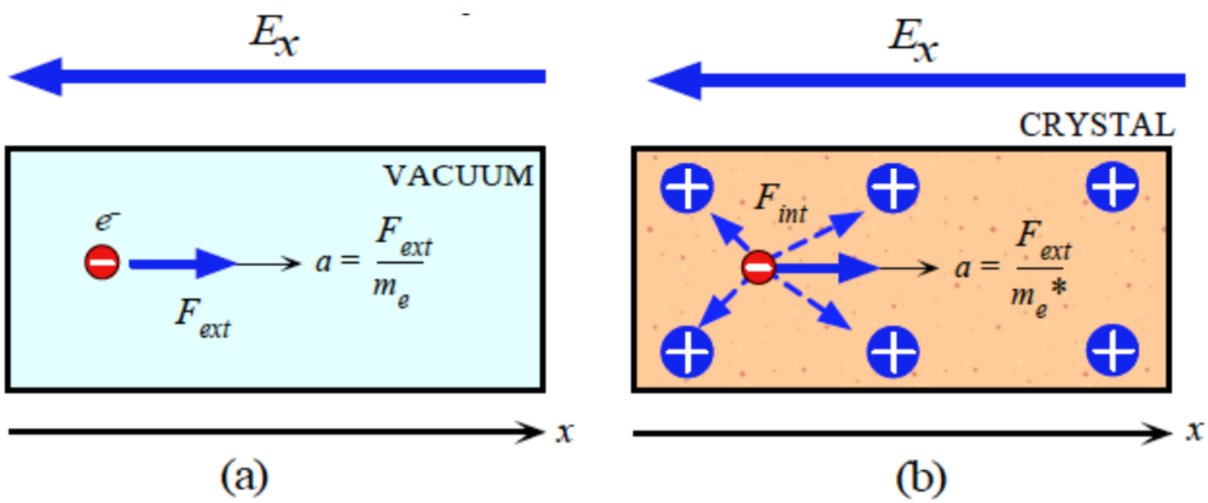


Figure 13.

The acceleration of an electron in a vacuum and a crystal is given by equations below:

$$a_v = \frac{F_{ext}}{m_e} \text{ (in a vacuum)} \qquad \text{............ (1)}$$

$$a = \frac{(F_{ext}+F_{int})}{m_e} = \frac{(F_{ext}-\vec{\nabla}V)}{m_e} = \frac{F_{ext}}{m_e^*} \qquad \text{(in a crystal)} \qquad \text{............. (2)}$$

where,

m_e is the mass of electron in a vacuum (9.1 × 10^{-31} kilograms)

m_e^* is the effective mass of electron in a crystal

$\vec{\nabla}V$ is the potential difference.

As a result, an electron in a crystal may behave as if it had a mass different from the free electron mass m_e. There are crystals in which the effective mass of the carriers is much larger or much smaller than m_e.

- If the electron is free, no potential barrier restricts the propagation of the electron wave (i.e. $\vec{\nabla}V$ = 0). So, the energy (E) represents the kinetic energy only:

As the electron momentum is $\mathrm{p} = m_e \mathrm{v} = \frac{\mathrm{h}}{\lambda} = \frac{2\pi\hbar}{\lambda} = \hbar\mathbf{k}$ ……… (3)

So, the electron energy is $E = \frac{1}{2} m_e v^2 = \frac{1}{2}\frac{p^2}{m_e} = \frac{\hbar^2}{2m_e}\mathbf{k^2}$ ……… (4)

where $\mathbf{k}$ is a wave vector of the electron.

Figure 14 shows the relationship between the electron energy and the momentum (wave vector $\mathbf{k}$) for a free electron.

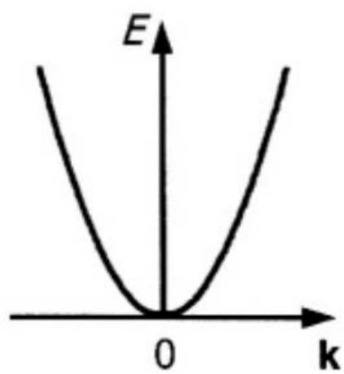


Figure 14.

- If the movement of electrons is in a crystal, we recall that, for a wave packet, the group velocity (v_g) can be expressed as

$$v_g = \frac{1}{\hbar}\frac{dE}{dk} \dots\dots\dots..(5)$$

and the acceleration a can be expressed as

$$a = \frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d^2E}{dk\,dt} = \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt} \quad \dots\dots\dots\dots(6)$$

dE/dk is known, and dk/dt can be evaluated from the expression $p = \hbar\mathbf{k}$

$$\frac{dp}{dt} = \hbar\frac{dk}{dt} \dots\dots\dots.(7)$$

where $\frac{dp}{dt} = \text{Force}$, thus,

$$a = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}\,F_{ext} \quad \dots\dots\dots\dots(8)$$

where F_{ext} is the force acting on an electron. By comparing Eq. (8) with an equation (2) that is identical to Newton's second law of motion, we can write

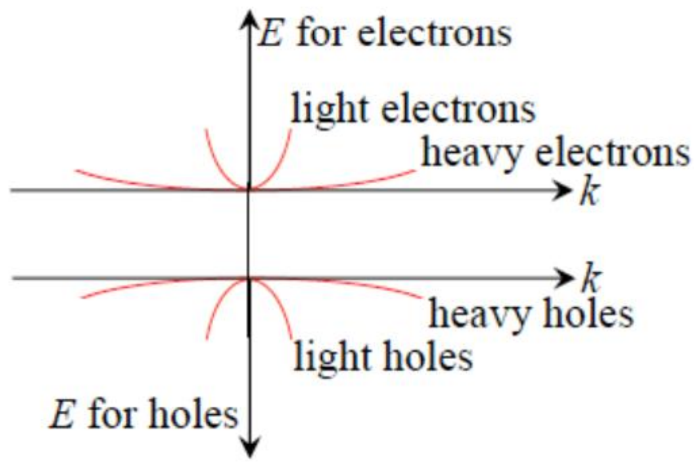
$$\frac{1}{m_e^*} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2} \quad \dots\dots\dots\dots.(9)$$

Or,

$$m_e^* = \hbar^2\left(\frac{d^2E}{dk^2}\right)^{-1} \quad \dots\dots\dots\dots.(10)$$

In other words, the electron effective mass is inversely proportional to the curvature of an electron energy band $E(k)$. This means that there are the *light-electron* band (larger curvature) and *heavy- electron* band (smaller curvature). In the valence band, similar considerations of the inverse dependence between the effective mass and energy band curvature indicate that there are the *light-hole* band (larger curvature) and *heavy-hole* band (smaller curvature), see Figure 15.

Figure 15.

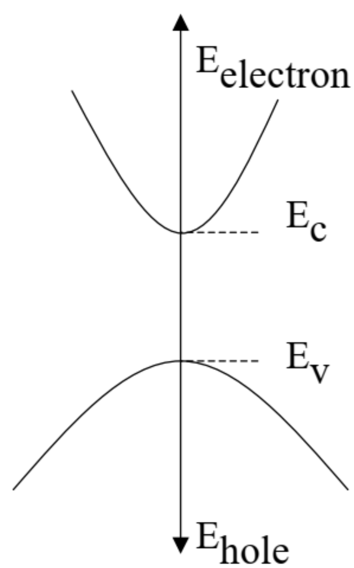


Note: the effective mass of hole (m_h^*) is also different in a crystal, and its value is often different than the effective mass value of the electron (m_e^*)

Parabolic Approximations of Bands

Thus, for parabolic bands, the electron will move much like a free particle with m_e, which is related to the curvature of the band. For nonparabolic bands, m_e is not constant and the curvature of the E–k relationship must be used to obtain the velocity and acceleration of the particle with energy E.

The shape of the bottom of the conduction band and the top of the valence band can be approximated by parabolas, which results in constant effective masses.



The energy in the conduction band is:

$$E = E_c + \frac{\hbar^2 k^2}{2m_e^*}$$

The energy in the valence band is:

$$E = E_v - \frac{\hbar^2 k^2}{2m_h^*}$$

where E_c is the conduction band energy, E_v is the valence band energy.