BAND THEORY

KRONIG & PENNY MODEL:

In metal there is regular arrangement of atoms, atoms having valence electron are mobile. After leaving valence electron atom become positively charged ion. Thus an atom may be regarded as an array of positive ion of lattice.

When the electric feild is applied on the metal then electron starts accelerating in one particular direction say along x-axis by gaining kinetic energy. On his journey it strikes the positive ion of lattice and gain additional kinetic energy. But at some distance apart a retardation force exist between electron and positive ion. This process will continue till the electric feild is applied on metal and kinetic energy changes into potential energy.

Notes: Thus, atom may be regarded as an square well potential. A array of metal is equivalent to periodic array of square well potential.

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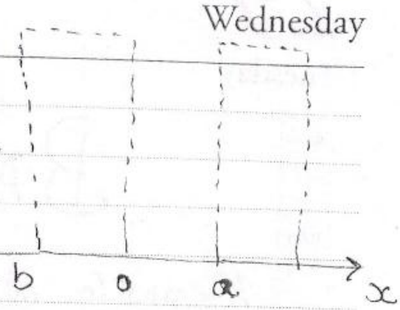

In the region $0 < x < a$, potential energy is min. but kinetic energy is maximum.

In the region $0 < x < -b$, potential energy is maximum and kinetic energy is minimum.

According, to quantum theory a particle having wave whose wavelength is defined as:

$$\lambda = \frac{h}{p} \quad \text{or} \quad p = \frac{h}{\lambda}$$

multiply and divide by 2π

$$p = \frac{h}{\lambda} \times \frac{2\pi}{2\pi} \qquad \left[\frac{2\pi}{\lambda} = k, \quad \frac{h}{2\pi} = \hbar \right]$$

$$p = \hbar k$$

Squaring both Sides

$$p^2 = \hbar^2 k^2 \quad -(1)$$

When the electric feild is applied on the metal then electrons gain kinetic energy E;

$$E = \frac{1}{2} m v^2 = \frac{p^2}{2m}$$

$$E = \frac{\hbar^2 k^2}{2m} \quad -(2)$$

Notes

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E - k Diagram

From the above equation it is clear that relation between E and k is parabolic.

$$E = \frac{\hbar k^2}{2m}$$

The parabolic nature between E and k is valid only in case of free electron. The energy is interrupted at different value of k so first we will find that value of k at the energy will interrupted.

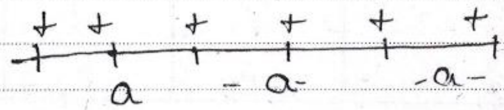
Consider that electron is incident normally on the plane of crystal lattice seperated by distance 'a'. Then Bragg condition is satisfied:

$$2d \sin\theta = n\lambda$$

$$2a = \pm n\lambda \qquad \left[\lambda = \frac{2\pi}{k}\right]$$

$$2a = \pm n \frac{2\pi}{k}$$

$$k = \pm \frac{n\pi}{a}$$



For $n = 1$, $k = \pm \frac{\pi}{a}$

For $n = 2$, $k = \pm \frac{2\pi}{a}$

For $n = 3$, $k = \pm \frac{3\pi}{a}$

OCTOBER 2009

SEPTEMBER 2009

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NOVEMBER 2009

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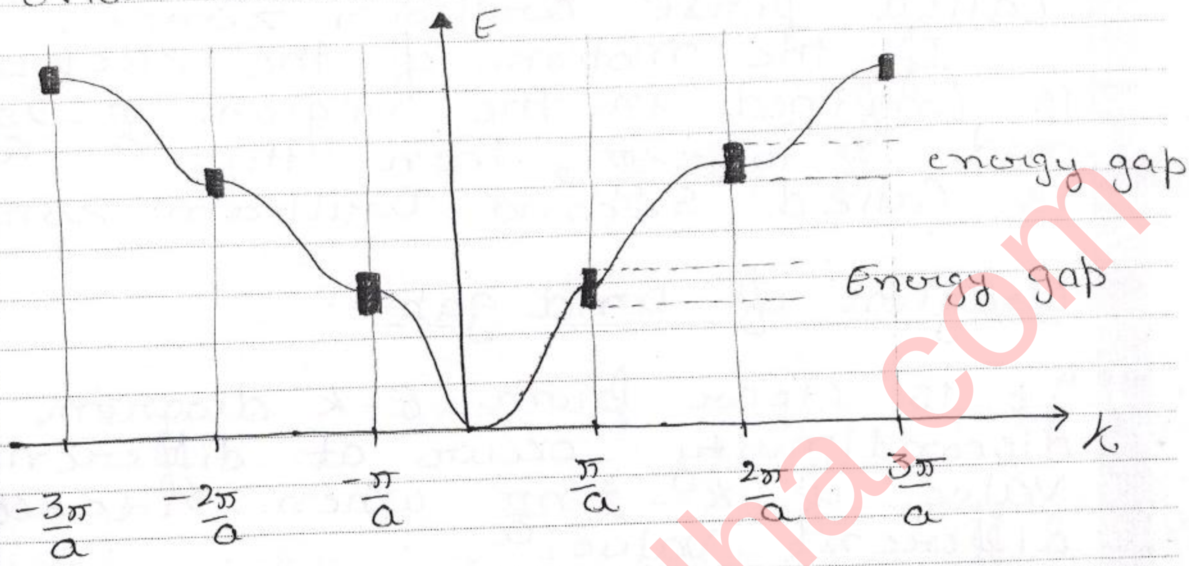
Learn a new skill. You might connect this with your main hobby or with your work. The mind and the body are one. To master a physical skill you need to develop a disciplined, lively mind to direct your hands and feet the way they should go.

Graph is plotted between Energy and wave number (k).



From the given graph it is clear that discontinuity occurs at different value of $k = \pm \frac{\pi}{a}, \pm \frac{2\pi}{a}$ ---

When electric feild is applied on the metal then kinetic energy is gain by electron which is not sufficient to overcome the potential. Thus the motion of the electron is confined in the region $-\frac{\pi}{a}$ to $\frac{\pi}{a}$.

Brillioun Zone

Notes

Since, discontinuity in E-k diagram occur at different value of k.

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The motion of electron is confined in the region $-\frac{\pi}{a}$ to $\frac{\pi}{a}$, this is called first Brillioun zone.

If the motion of the electron is confined in the region $\frac{\pi}{a}$ - $\frac{2\pi}{a}$ and $-\frac{\pi}{a}$ to $-\frac{2\pi}{a}$, then this is called second brillioun zone.

Origion of band gap

It is clear from E-k diagram that discontinuity occur at different value of $k = \pm \frac{n\pi}{a}$ when n takes different value.
Motion of electron is confined in the region $-\frac{\pi}{a}$ to $\frac{\pi}{a}$. There occur a discontinuity in the energy gap of electron which is called band gap or forbidden gap.
Now there allowed an onother energy zone which occur at value of $k = \frac{2\pi}{a}$, That is band gap occurs at different value of k.

EFFECTIVE MASS OF ELECTRON:

A free electron has well defined mass and obeys Newton's law when acted upon by an external electric feild. But if the electron is placed in periodic array of Crystal lattice then the behaviour in external electric feild is different, from that of free electron.

Acc. to Shrodinger, velocity of particle v is equivalent to group velocity V_g

$$v = V_g = \frac{d\omega}{dk}$$

ω - angular frequency, k - wave number

But according to quantum theory of mechanics, energy is given as:

$$E = h\nu$$

multiply and divide by 2π

$$E = \frac{h}{2\pi} \cdot 2\pi\nu = \hbar\omega$$

Differentiate the equation

$$\frac{dE}{dk} = \hbar \frac{d\omega}{dk}$$

$$\frac{1}{\hbar}\frac{dE}{dk} = v$$

Notes: Now, when electric feild is applied is applied on the metal, force experience by electron

$$F = -eX_c$$

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Work done in displacing body through small distance dx

$$dE = dw = -eX_e\,dx \qquad \left[v = \frac{dx}{dt}\right]$$

$$dE = -eX_e\,v\,dt$$

$$dE = -eX_e \cdot \frac{1}{\hbar}\frac{dE}{dk}\,dt$$

Multiply by dk on left side and divide also

$$\frac{dE}{dk}\cdot\frac{dk}{dt} = -eX_e \cdot \frac{1}{\hbar}\frac{dE}{dk} \quad -(1)$$

Now, $a = \frac{dv}{dt} = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{dE}{dk}\right)$

$$= \frac{1}{\hbar}\frac{d^2E}{dk^2}\cdot\frac{dk}{dt}$$

$$= \frac{1}{\hbar}\frac{d^2E}{dk^2}\cdot -eX_e\frac{1}{\hbar}$$

$$= \frac{1}{\hbar^2}\frac{d^2E}{dk^2}\,-eX_e \quad -(2)$$

Now, $F = ma = -eX_e$

$$a = \frac{-eX_e}{m} \quad -(3)$$

Notes

On comparing (2) and (3)

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$$\frac{1}{m} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}$$

$$m = \frac{\hbar^2}{d^2E / dk^2}$$

This is called effective mass of electron.

HALL EFFECT:

If a current carrying conductor is placed in a magnetic feild then voltage is developed perpendicular to both direction of magnetic feild and current. This is called hall effect.

Consider a current carrying conductor of thickness 't' and width 'b' placed in a magnetic feild. Then voltage is applied along x-axis then current flows in positive direction of x-axis. Due to this current electrostatic feild is also developed along x-axis that causes the electrons to accelerate towards negative direction of x-axis. In the presence of magnetic feild, magnetic lorentz force act that is:

$$F_m = V_d (B \cdot q)$$

$q = -e$, $V_d = -V_d \hat{i}$, $B = B_z \hat{k}$

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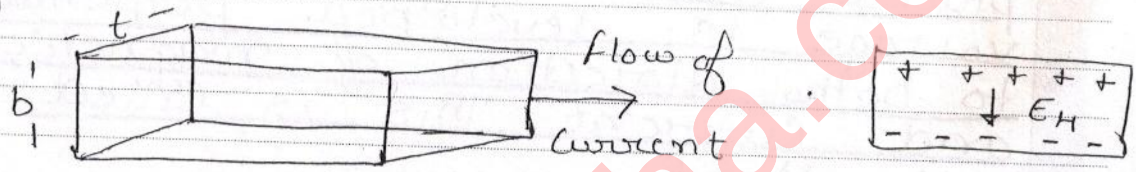
$$F_m = -e v_d B_z$$

This force causes the electron to accelerate towards negetive direction of y-axis. Electrons are collected at the surface and potential difference is induced along negative y-axis which causes a current to flow that opposes magnetic lorentz force.



$$-e v_d B_z = -e E_H$$

$$v_d = \frac{E_H}{B_z} \quad -(1)$$

If the substance contains n no. of electron having charge e and drifted through velocity v_d.

$$J_x = -n e v_d$$

$$J_x = -ne \frac{E_H}{B_z}$$

$$E_H = -\frac{1}{ne} J_x B_z$$

$\left[R_H = -\frac{1}{ne} \right.$ because charge carrier are electron

$$E_H = R_H J_x B_z$$

R_H (Hall effect coefficient)

But $E_H = \frac{V_H}{b}$

$\frac{V_H}{b} = R_H J_x B_z$

$R_H = \frac{V_H}{b J_x B_z}$

Since, b is width of current carrying conductor and t is the thickness so crossectional area will be bt. The current density $J_x = \frac{I_x}{bt}$

$R_H = \frac{V_H\, bt}{b I_x B_z} = \frac{V_H t}{I_x B_z}$

Importance:
Hall effect can be used to find out mobility of electron.

$\mu = \frac{V_d}{E_H}, \quad \mu E_H = V_d$

But $E_H = V_d B_z$

$E_H = \mu E_H B_z$ Compare with $R_H J_x B_z$

$\mu E_H B_z = R_H J_x B_z \quad [J_x = \sigma E_H]$

$\mu = \sigma R_H$

Notes

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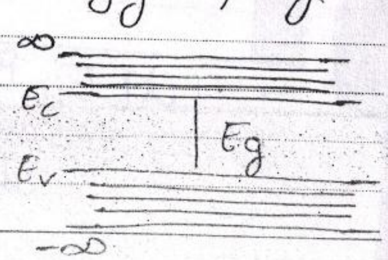
EFFECT OF FERMI ENERGY

The band structure of insulators at 0K is same as that of intrinsic semiconductor. Filled valence bond and empty conduction bond is seperated by energy gap E_g therefore electrical conduction doesn't take place. If the temperature is increased then electron starts moving from filled valence bond to conduction bond and electrical conduction takes place. The number of electron in conduction bond and holes in valence bond are same.

First of all calculate the number of electrons moves from conduction bond to valence bond. In making these calculations energy is taken from top of valence bond. Effective mass of electron in m_e and hole is m_h.

The number of electron present in conduction bond has energy lying from E_c to ∞ and holes in valence bond has $-\infty$ to E_v.



According to Concept of fermi energy, total no of electrons present in conduction band is n_c.

$$dn_c = f(E) \cdot D(E)\, dE$$

$$f(E) = \frac{1}{1+e^{(E-E_F)/kT}}$$

Since, $e^{E-E_F/kT} >>> 1$ one can neglected

$$= \frac{1}{e^{(E-E_F)/kT}}$$

D(E) is density of state at bottom of the conduction band.

$$D(E) = \frac{4\pi}{h^3}(2m_e)^{3/2}\cdot(E-E_c)^{1/2}$$

$$n_c = \int dn_c = \int_{E_c}^{\infty} \frac{4\pi}{h^3}(2m_e)^{3/2}\cdot(E-E_c)^{1/2}\cdot e^{-(E-E_F)/kT}$$

$$= \frac{4\pi}{h^3}(2m_e)^{3/2}\cdot e^{E_F/kT}\int_{E_c}^{\infty}(E-E_c)^{1/2}\cdot e^{-(E-E_c)/kT}\cdot e^{-E_c}$$

$$= \frac{4\pi}{h^3}(2m_e)^{3/2}\cdot e^{E_F-E_c/kT}\int_{E_c}^{\infty} e^{-(E-E_c)/kT}\cdot(E-E_c)^{1/2}$$

Notes

Put $\frac{E-E_c}{kT} = x$

$$dE = kT\, dx$$

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when $E=\infty$, $x=\infty$

When $E = E_c$, $x = 0$

$$(kT)\int e^{-x}\cdot(kT)^{1/2}\cdot x^{1/2}\,dx$$

$$(kT)^{3/2}\cdot\Gamma\tfrac{1}{2} = (kT)^{3/2}\cdot\sqrt{\pi}$$

$$\therefore n_e = \frac{4\pi}{h^3}\cdot(2m_e)^{3/2}\cdot e^{\frac{E_F - E_C}{kT}}\cdot(kT)^{3/2}\cdot\sqrt{\pi} \quad -(1)$$

Now, Density of hole in Valence band

$$f_c(E) + f_h(E) = 1$$

$$f_h(E) = 1 - f_e(E)$$

$$F_h(E) = 1 - \frac{1}{1+e^{(E-E_F)/kT}} = e^{(E-E_F)/kT}$$

$$n_h = \int \frac{4\pi}{h^3}(2m_h)^{3/2}\cdot e^{(E-E_F)/kT}\cdot(E_v - E)^{1/2}$$

$$= \frac{4\pi}{h^3}(2m_h)^{3/2}\cdot e^{-E_F/kT}\int (E_v - E)^{1/2}\cdot e^{-(E_v - E)/kT}$$

$$= \frac{4\pi}{h^3}(2m_h)^{3/2}\cdot e^{\frac{E_v - E_F}{kT}}\cdot(kT)^{3/2}\cdot\sqrt{\pi}$$

(On Solving, Simillarly.)

In intrinsic Semiconductor, no of holes = no of electrons.

$$\left(\frac{2m_c}{2m_h}\right)^{3/2} = e^{\frac{E_F - E_c - E_v + E_F}{kT}}$$

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taking log on both Sides

$$\frac{3}{2} \log \frac{m_e}{m_h} = 2E_F - E_V - E_C$$

if mass of e^- and hole is Same

then $0 = E_V + E_C - 2E_F$

$$E_F = \frac{E_V + E_C}{2}$$

Thus, fermi level lies exactly half of the valence band and Conduction band.

Notes

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