

Q What is Kronig-Penny model? What does it represent?

Ans:- It is the model for electron in one-dimensional periodic potential. The possible states that the e^- can occupy are determined by Schrödinger equation.

It represents simple one-dimensional periodic potential yields energy bands as well as energy band gaps.

The Potential assume is
$$V(x) = \begin{cases} 0, & 0 < x < a \\ V_0, & -b < x < 0. \end{cases}$$

We need to solve Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{nk}(x) + V(x) \psi_{nk}(x) = E_{nk} \psi_{nk}(x).$$

(Q) What is effective mass? How is it defined in E vs k diagram?

(Ans) $F_{\text{total}} = F_{\text{ext}} + F_{\text{int}} = m^* a$

$$F_{\text{ext}} = m^* a.$$

here m^* is effective mass, takes into account the particle mass and also the effect of internal forces

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

$$F = ma = -eE$$

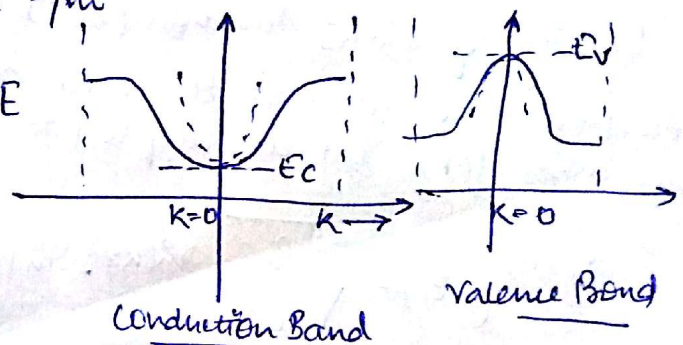
$$a = \frac{-eE}{m}$$

$$\frac{d^2 E}{dk^2} = 2C_1$$

$$\Rightarrow \frac{1}{\hbar^2} \cdot \frac{d^2 E}{dk^2} = \frac{2C_1}{\hbar^2}$$

$$\Rightarrow \left[\frac{1}{\hbar^2} \cdot \frac{d^2 E}{dk^2} = \frac{2C_1}{\hbar^2} \approx \frac{1}{m^*} \right]$$

$$a = \frac{-eE}{m^*}$$

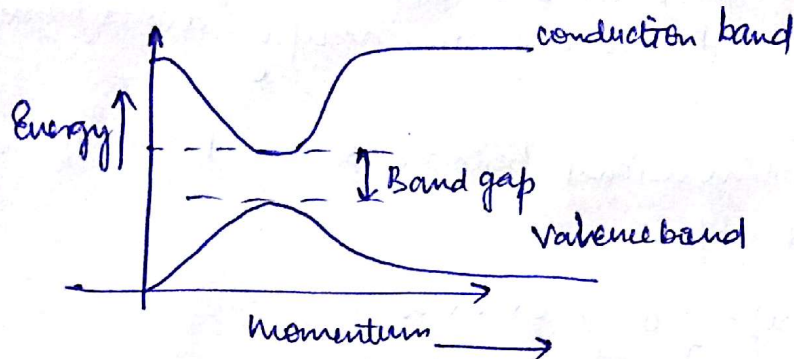


E vs k diagram

③ What is direct & indirect band gap Semiconductor? Page no: -02

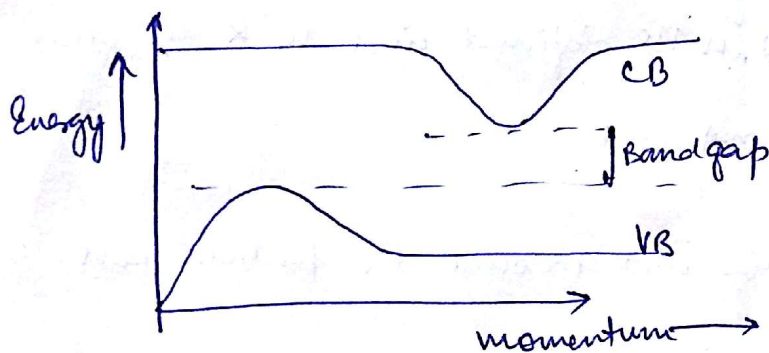
Ans: Direct bandgap semiconductor.

In direct bandgap semiconductor, top of valence band and bottom of conduction band occur at same value of ~~low~~ momentum.



Indirect bandgap semiconductor.

The maximum energy of valence band occurs at different value of momentum to the minimum in conduction band energy.

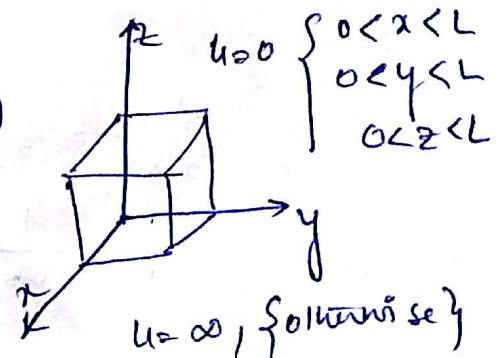


④ Density of states function (DOS)

Electrons are allowed to move relatively freely in conduction band of semiconductor, but are confined to crystal.

$$\Psi(n_x, n_y, n_z) = \sqrt{\frac{q}{L^3}} \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

$$E = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2)$$



⑤

Fermi-level at $T > 0K$



$$E_f = \frac{\hbar^2 k_f^2}{2m}$$

max value of energy for filled states is known as E_f

density of filled states = $\frac{N}{V} = \frac{1}{3\pi^2} \left(\frac{2mE_f}{\hbar^2} \right)^{3/2}$

⑤ Relation between DOS and Energy

Page no: -03

$$g(E) = \frac{4\pi (2m)^{3/2}}{\hbar^3} \sqrt{E} \rightarrow \text{It is the density of quantum state per unit volume of the crystal.}$$

⑥ Fermi Dirac probability function.

max of 1 particle is allowed in each quantum state (by Pauli exclusion principle). There are g_i ways of choosing where to place the first particle, $(g_i - 1)$ ways for second particle and so on.

Total no of ways of arranging N_i particles in i th level N_i where $N_i \leq g_i \rightarrow g_i (g_i - 1) \dots (g_i - N_i + 1) = \frac{g_i!}{(g_i - N_i)!}$

Actual number of independent ways of arranging N_i particles in i th level is $w_i = \frac{g_i!}{N_i! (g_i - N_i)!}$

⑦ Fermi energy

The energy below which all states are filled with electrons and above which all the states are empty at $T > 0K$.

⑧ Effective mass

$$m^* = \left(\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \right)^{-1}$$

$$\frac{d^2 E}{dk^2} \text{ of curve A} > \frac{d^2 E}{dk^2} \text{ of curve B}$$

$$\Rightarrow m^* \text{ of curve A} < m^* \text{ of curve B}$$

So, B will have heavier effective mass.

$$\textcircled{9} \quad E_v - E = \frac{\hbar^2 k^2}{2m} \quad k = 0.08 (\text{\AA}^{-1}) = 0.08 \times 10^{10} = 8 \times 10^8 \text{ m}^{-1}$$

from curve A \Rightarrow

$$(0.025) \times (1.6 \times 10^{-11}) = \frac{(8 \times 10^8)^2 (1.054 \times 10^{-34})^2}{2m}$$

$$m = \frac{(8 \times 10^8)^2 (1.054 \times 10^{-34})^2}{2 \times 0.025 \times 1.6 \times 10^{-19}}$$

Page no: 04

$$= \frac{7.1 \times 10^{-51}}{0.08 \times 10^{-19}} = 88.75 \times 10^{-32}$$

$$m = 8.88 \times 10^{-31} \text{ kg}$$

$$\Rightarrow m/m_0 = \frac{8.8 \times 10^{-31}}{9.1 \times 10^{-31}} = 0.975$$

for curve B \rightarrow

$$(0.3)(1.6 \times 10^{-19}) = \frac{(8 \times 10^8)^2 (1.054 \times 10^{-34})^2}{2m}$$

$$m = \frac{(8 \times 10^8)^2 (1.054 \times 10^{-34})^2}{2 \times 0.3 \times (1.6 \times 10^{-19})}$$

$$= 7.4 \times 10^{-32} \text{ kg}$$

$$\frac{m}{m_0} = \frac{7.4 \times 10^{-32}}{9.1 \times 10^{-31}} = 0.74$$

(10) Fermi energy level = 6.25 eV

T = ?

1% Probability

0.30 eV below Fermi energy level will not contain an $e^- = 6.25 - 0.30 = 5.95 \text{ eV}$

Probability that it will not contain $e^- \Rightarrow$

$$1 - f_F(E) = 1 - \frac{1}{1 + e^{\frac{E - E_f}{kT}}}$$

$$0.01 = 1 - \frac{1}{1 + e^{(5.95 - 0.25)/kT}}$$

$$\frac{1}{1 + e^{-0.3/kT}} = 0.99$$

$$1 + e^{-\frac{0.3}{kT}} = \frac{1}{0.99}$$

$$kT = 0.06529 \text{ eV}$$

$$T = \frac{0.0652}{k}$$

$$T = 756 \text{ K}$$

(11) $T = 300\text{ K}$
 $3kT$ above fermi energy

$$f_f(E) = \frac{1}{1 + e^{\frac{E - E_F}{kT}}} = \frac{1}{1 + e^{3kT/kT}}$$

$$f_f(E) = \frac{1}{1 + 20.09} = 0.0474$$

$$= 4.74\%$$

(12) no. of quantum states = ?
 between $E_c + E_c - kT$ at $T = 300\text{ K}$

$\text{Si} \rightarrow$

$$g_c(E) dE = \frac{4\pi (2m_n^*)^{3/2}}{h^3} \int_{E_c}^{E_c + kT} \sqrt{E - E_c} dE$$

$$= \frac{4\pi (2m_n^*)^{3/2}}{h^3} \left(\frac{2}{3} \right) (E - E_c)^{3/2} \Big|_{E_c}^{E_c + kT}$$

(14) DOS per unit volume

$$\int_0^1 g(E) dE = \frac{4\pi (2m)^{3/2}}{h^3} \int_0^1 \sqrt{E} dE$$

$$\approx \frac{4\pi (2m)^{3/2}}{h^3} \times \frac{2}{3} E^{3/2}$$

$$N = 4.5 \times 10^{27} \text{ m}^{-3}$$

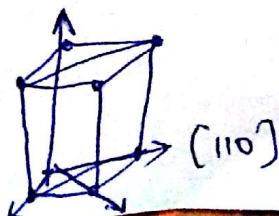
$$\Rightarrow N = 4.5 \times 10^{21} \text{ states/cm}^3$$

(15) lattice constant = a

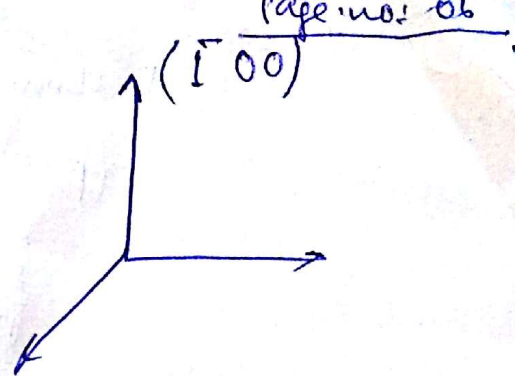
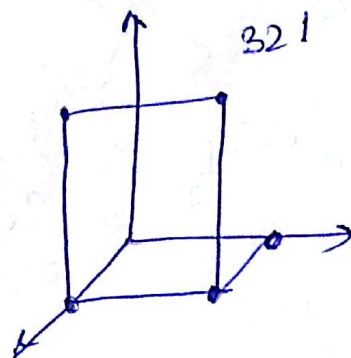
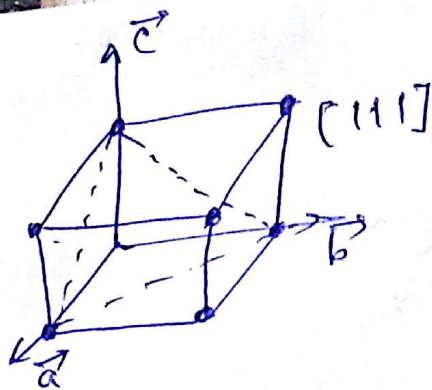
- (e) 110
- (ii) 111
- (iii) 220
- (iv) 321
- (v) ~~100~~ $\bar{1}00$
- (vi) $\bar{1}11$

(16) $[110]$ $[111]$ $[220]$ $[321]$

(1) $[110]$



P.T.O.



(17) Surface density of atoms (Si)
 (a) (100) plane (b) (110) plane (c) (111) plane

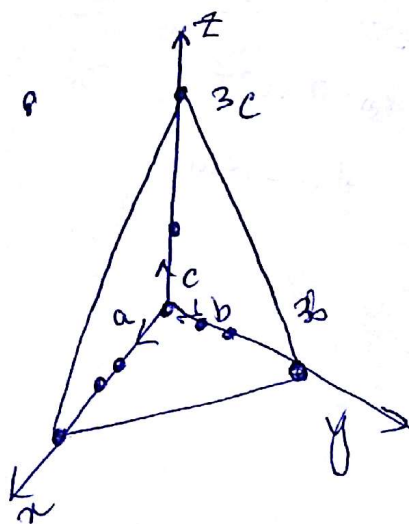
Surface density = $\frac{\text{No. of atoms}}{\text{Area of LP}}$

(a) (100) plane ; $S.D = \frac{2 \text{ atoms}}{(5.43 \times 10^{-8})^2} = 6.78 \times 10^{14} \text{ cm}^{-2}$

(b) (110) plane ; $S.D = \frac{4 \text{ atoms}}{\sqrt{2} (5.43 \times 10^{-8})^2} = 9.59 \times 10^{14} \text{ cm}^{-2}$

(c) (111) plane ; $S.D = \frac{4 \text{ atoms}}{\sqrt{3} (5.43 \times 10^{-8})^2} = 7.83 \times 10^{14} \text{ cm}^{-2}$

(18)



(a) Miller indices : $[3, 3, 3]$
 (b) Miller indices = $[3, 2, 2]$