1. **Quantum Free Electron Theory (QFET)** **[10 M]**
   a) Compare and contrast the postulates of classical free electron theory with that of quantum free electron theory. [BT 1][6 M]
   b) What are the merits of quantum free electron theory? [BT 1][2 M]
   c) What are the demerits of quantum free electron theory? [BT 1][2 M]

Module bank solutions

PART - A

① Quantum free electron theory

a) Compare and contrast the postulates of classical free electron theory with that of quantum free electron theory

Solution:

Type	CFET	QFET
Nature of electron (1)	Particle Electron is a classical particle with mass m and charge $-e$ with energy E and ~~veloct~~ momentum p	Wave Electron is a quantum wave with wavevector k and angular frequency ω with energy $E = \hbar\omega$ and momentum $p = \hbar K$.
Kinematics (1)	Independent electron approximation Electrons are independent i.e. mutual repulsion between them is ignored	Also electron is a fermion with spin $\frac{1}{2}$ and obeys Paulis' exclusion principle. → Also IE approximation is considered.
Dynamics	Free electron approximation Electrons are	Also FE approximation

	free and move in an infinite potential well	is considered.
(2)	Electrons undergo collisions ~~to~~ with ions to thermalize leading to thermal motion ~~I~~ between collisions. Dynamics governed by Lorentz force $\vec{F}_e = -e(\vec{E} + \vec{V} \times \vec{B})$ leading to drift motion	Ions are considered as collective and quantum of vibration is called phonon. Interaction of electron and phonon leads to thermalization
Thermodynamics (2)	The thermalization is governed by Maxwell Boltzmann statistics	Thermalization is governed by Fermi Dirac statistics

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b) What are the merits of QFET?

Solution:

1 - Explanation of electrical conductivity
- thermal conductivity

1 - Heat capacity

c) What are the demerits of QFET?

Solution

1 - Classification of condensed matter into metals, semiconductors and insulators

1 - Occurrence of positive Hall coefficient in some metals like Zn. (anomalous Hall coefficient)

2. Fermi-Dirac Distribution **[10 M]**

a) Plot the probability of occupancy of energy level in the case of Maxwell-Boltzmann distribution and Fermi-Dirac distribution at
   i. $T = 0K$,
   ii. $T \neq 0K$, and
   iii. $T = \infty\, K$ [BT 2][2 M]

b) Five free electrons exist in a three-dimensional infinite potential well with all three widths equal to $a = 12$ Å.
   i. Determine the Fermi energy level at $T = 0K$.
   ii. Repeat part (i) for 13 electrons. [BT 3][4 M]

c) Fermi level of a metal is $6.25\ eV$ and electrons in this material follow the Fermi-Dirac distribution. Calculate the temperature at which there is 1% probability that a state $0.30\ eV$ below the Fermi energy level will **not** contain an electron. [BT 3][4 M]

② Fermi - Dirac distribution

a) Plot the probability of occupancy of energy level in the case of Maxwell- Boltzmann distribution and Fermi-Dirac distribution at

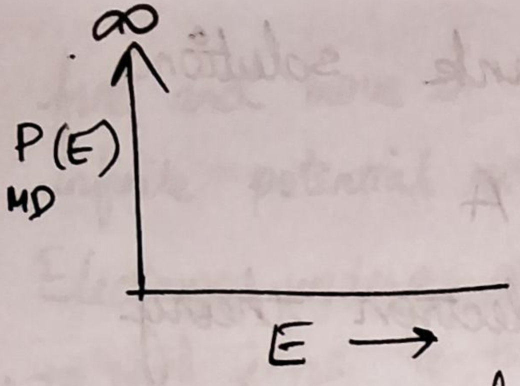
(i) $T = 0K$

(ii) $T \neq 0K$

(iii) $T = \infty K$

Solution :

MB	FD
0.5 $P_{MB}(E) = e^{\frac{-E}{k_BT}}$	$P_{FD}(E) = \frac{1}{1+\exp\left(\frac{E-E_F}{k_BT}\right)}$ where E_F = Fermi level
(i) $T = 0K$	
$P_{MB}(E) = e^{\frac{-E}{0}}$ 0.5 $= e^{-\infty}$ $= 0$ if $E \neq 0$ @ $E = 0$ $P_{MB}(E=0) = e^{-\frac{0}{0}}$ = indeterminate form But particles need to occupy some level, all the particles occupy the ground state level.	$P_{FD}(E) = \frac{1}{1+\exp\left(\frac{E-E_F}{0}\right)}$ @ $E > E_F$ $P_{FD}(E) = \frac{1}{1+\exp\left(\frac{+ve}{0}\right)}$ $= \frac{1}{1+\infty}$ $= 0$ @ $E < E_F$ $P_{FD}(E) = \frac{1}{1+\exp\left(\frac{-ve}{0}\right)}$ $= \frac{1}{1+0}$ $= 1$



Form is Dirac delta function

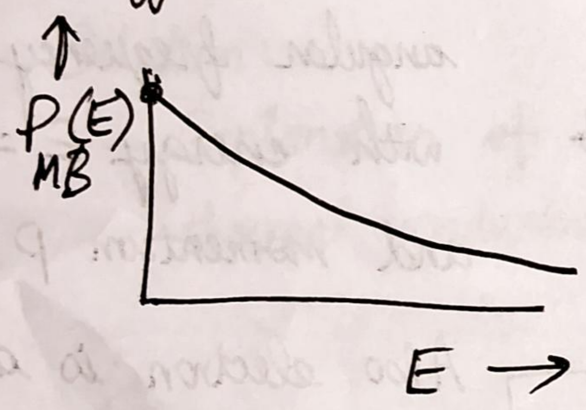
$$P_{MB}(E) = \delta(E)$$

(ii) T ≠ 0K

$$P_{MB}(E) = e^{-\frac{E}{k_BT}}$$

0.5

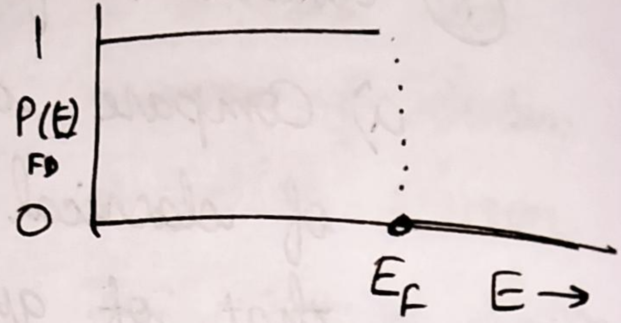
Highest occupancy is for ground state and occupancy reduces exponentially for higher energy levels.



@ E = E_F

$$P_{FD}(E) = \frac{1}{1+\exp\left(\frac{0}{0}\right)}$$

indeterminate form



$$P_{FD}(E) = \frac{1}{1+\exp\left(\frac{E-E_F}{k_BT}\right)}$$

@ E >> E_F

$$P_{FD}(E) = \frac{1}{1+\exp\left(\frac{+ve}{+ve}\right)}$$

$$\simeq \frac{1}{1+\infty}$$

$$= 0$$

@ E << E_F

$$P_{FD}(E) = \frac{1}{1+\exp\left(\frac{-ve}{+ve}\right)}$$

$$\simeq \frac{1}{1+0}$$

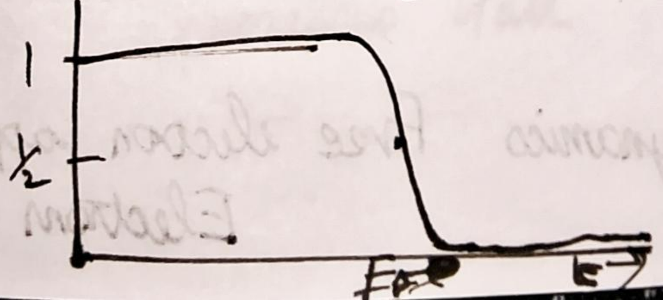
$$= 1$$

@ E = E_F

$$P_{FD}(E) = \frac{1}{1+\exp\left(\frac{0}{+ve}\right)}$$

$$= \frac{1}{1+1}$$

$$= \frac{1}{2}$$

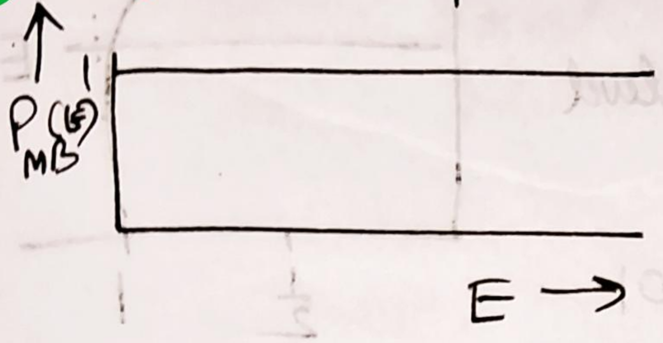


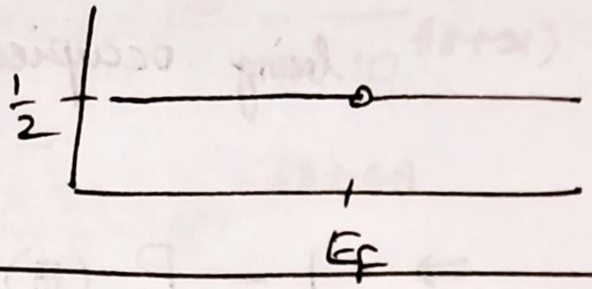
(iii) $T = \infty\,K$

$$P_{MB}(E) = e^{\frac{-E}{\infty}} = e^{0} = 1$$

$$P_{FD}(E) = \frac{1}{1+\exp\left(\frac{E-E_F}{\infty}\right)} = \frac{1}{1+\exp(0)} = \frac{1}{2}$$

0.5





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b) Five electrons exist in a three-dimensional infinite potential well with all three widths equal to $a = 12\,\mathring{A}$

(i) Determine the Fermi energy level @ $T = 0K$

(ii) Repeat part (i) for 13 electrons.

Solution:

For a particle in a 3D infinite potential cube well, of ~~cube~~ width a, the wavefunction is given by

$$\psi_{n_1,n_2,n_3}(x) = \left(\sqrt{\frac{2}{L}}\right)^3 \sin\left(\frac{n_1\pi x}{a}\right)\sin\left(\frac{n_2\pi y}{a}\right)\sin\left(\frac{n_3\pi z}{a}\right)$$

with energy of the level given by

(1)

$$E_{n_1,n_2,n_3} = \frac{(n_1^2+n_2^2+n_3^2)h^2}{8ma^2}$$

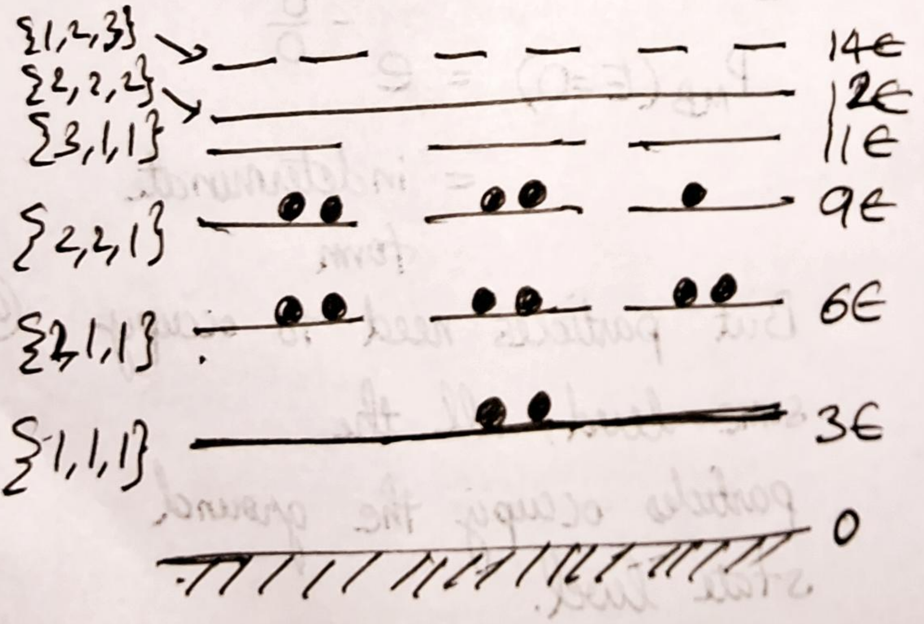
The levels are given by

n_1	n_2	n_3	E_{n_1,n_2,n_3}	degeneracy
1	1	1	$3E$	1

2	1	1	6ϵ	3
1	2	1		
1	1	2		
2	2	1	9ϵ	3
1	2	2		
2	1	2		
2	2	2	12ϵ	1
3	1	1	~~11ϵ~~	
1	3	1	11ϵ	3
1	1	3		
1	2	3	14ϵ	6
1	3	2		
2	3	1		
2	1	3		
3	1	2		
3	2	1		

(1)

Here $\epsilon = \frac{h^2}{8ma^2}$

Energy levels sketch

Here, spin degeneracy is also considered

For 5 electron system,
max energy of filled level is 6ϵ

$\therefore E_F = 6\epsilon$

Now $$\epsilon = \frac{h^2}{8ma^2} = \frac{(6.6\cdot10^{-34})^2}{8\cdot9.1\cdot10^{-31}\cdot(1.2\cdot10^{-9})^2}$$

$$= \frac{\overset{1.1}{\cancel{\overset{2.2}{\cancel{6.6}}}}\cdot\overset{1.1}{\cancel{\overset{2.2}{\cancel{6.6}}}}\cdot10^{-68}}{\underset{2}{\cancel{8}}\cdot\cancel{9.1}\cdot1.44\cdot10^{-(18+31)}}$$

$$= \frac{1.21}{2.88}\,10^{-68+49}$$

$$\epsilon\ (\text{in eV}) \approx \frac{\overset{0.4}{\cancel{1.21}}\cdot10^{-19}}{3\cdot1.6\cdot10^{-19}}$$

$$= 0.25\ \text{eV}$$

So $E_F = 6\cdot0.25$

$E_F = 1.5\ \text{eV}$ (1)

For 13 electron system
max energy of filled level is 9ϵ

$\therefore E_F = 9\epsilon$

$= 9\cdot0.25$

$E_F = 2.25\ \text{eV}$ (1)

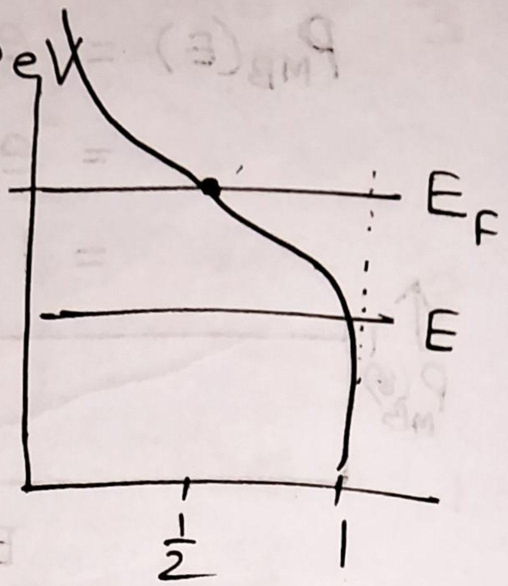
c) $E_F = 6.25$ eV of metal.
Electrons follow Fermi – Dirac distribution
Calculate temperature at which there is 1% probability that a state 0.30 eV below the Fermi energy level will not contain an electron.

Solution :

Let temperature be $T_?$

Energy of level considered is

(1) $E = E_F - 0.30\,\text{eV}$



Prob of level being empty =

1 − Probability of level being occupied

$= 0.01$

$\Rightarrow 1 - P_{FD}(E) = 0.01$

(1) $\Rightarrow 1 - \dfrac{1}{1+\exp\left(\frac{E-E_F}{k_B T_?}\right)} = 0.01$

$\Rightarrow \dfrac{1}{1+\exp\left(\frac{E-E_F}{k_B T_?}\right)} = 1 - 0.01 = 0.99$

$\Rightarrow 1+\exp\left(\frac{E-E_F}{k_B T_?}\right) = \dfrac{1}{0.99} = 1.0101$

$\Rightarrow \exp\left(\frac{E-E_F}{k_B T_?}\right) = 1.0101 - 1 = 0.0101$

$\Rightarrow \dfrac{E-E_F}{k_B T_?} = \ln(0.0101) = -4.595$

But $E - E_F = -0.30\,\text{eV}$

$\Rightarrow \dfrac{\cancel{-}0.30\,\text{eV}}{k_B T_?} = \cancel{-}4.595$

(1) $\Rightarrow k_B T_? = \dfrac{0.30}{4.595} = 0.0652\,\text{eV}$

Now $k_B T_{300} \rightarrow 0.0259\,\text{eV}$

$k_B T_? \rightarrow 0.0652\,\text{eV}$

$$\Rightarrow \frac{T_2}{T_{300}} = \frac{0.0652}{0.0259} = 2.52$$

$$\Rightarrow T_2 = 2.5 \cdot 300$$ (1)

$$T_2 = 756\ K$$

3. Electronic specific heat of solids **[10 M]**

a) Define specific heat of a material. What is its SI unit? [BT 1][2 M]

b) Specific heat of mercury ($^{200}_{80}Hg$) is $0.14\,J\,g^{-1}K^{-1}$. Report its specific heat in SI units. [BT 1][2 M]

c) Derive the expression for specific heat capacity from classical free electron theory and quantum free electron theory. [BT 4][6 M]

③ Electronic specific heat of solids

a) Define specific heat of a material. What is its SI unit?

Solution:

Specific heat is defined as the rate of change of energy E with temperature T per unit mole of material

$$C = \frac{dE}{dT} \quad (1)$$

$$\therefore \text{SI unit } [C] = \left[\frac{E}{T} \cdot \frac{1}{\text{mole}}\right] \quad (1)$$

$$= J\,K^{-1}\,mol^{-1}$$

b) Specific heat of mercury ~~is~~ $\left({}^{200}_{80}Hg\right)$ is $0.14\ J\,g^{-1}K^{-1}$. Report its specific heat in SI units.

Solution:

$$C_{Hg} = 0.14\ J\,g^{-1}\,K^{-1}$$

means Hg requires 0.14 J to raise its temperature by 1K for 1 gm of mercury.

(1) 1 mole of Hg ~~contains~~ weighs 200gm ~~of~~.

So 200 gm requires 0.14J × 200 to raise temperature by 1K.

(1) $\therefore C_{Hg} = 0.14 J \cdot 200 \ K^{-1} mol^{-1}$

$= 28 \ J \ mol^{-1} K^{-1}$.

c) Derive the expression for specific heat capacity from CFET and QFET.

Solution :

(i) From CFET

Average Kinetic energy of electron at temperature T is $\epsilon = \frac{3}{2} K_B T$.

Average energy of N_A electrons at T is

$$E = N_A \epsilon$$

$$= \frac{3}{2} K_B N_A T$$

Since $K_B N_A = R$

$$E = \frac{3}{2} RT$$

Now specific heat is

$$C = \frac{dE}{dT}$$

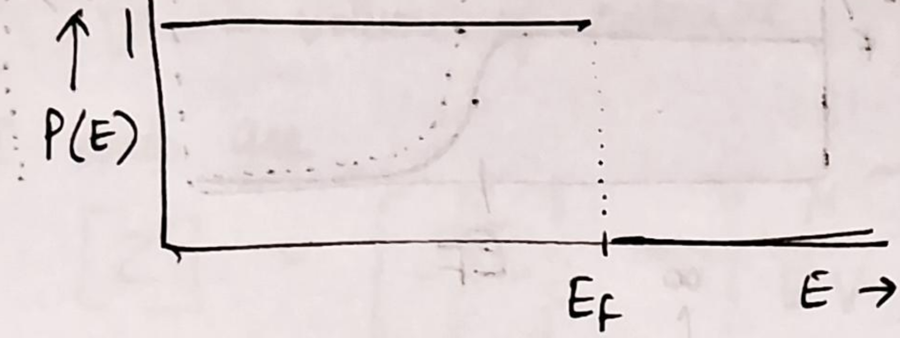
$$\Rightarrow C = \frac{d\cancel{\epsilon}}{dT}\left(\frac{3}{2}RT\right)$$

$$\Rightarrow \boxed{C = \frac{3}{2}R}$$

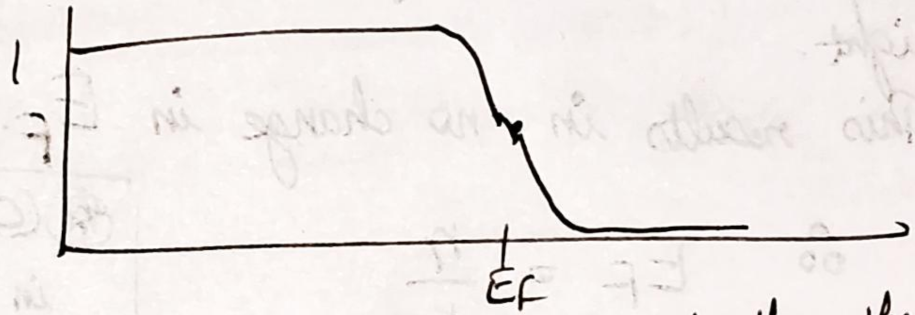
(2)

(ii) From QFET

At $T = 0K$, all the electrons occupy levels below Fermi energy level



At $T \neq 0K$,
thermalization leads to a fraction of electrons occupying higher levels than E_F. However not only the electrons whose energy ~~less than~~ lesser than K_BT below Fermi level participate in the thermalization and their energy rises by not more than K_BT above Fermi level.



The net increase of energy of the thermalized electrons is $K_BT = \epsilon_{thermal}$

The fraction of electrons that get thermalized is of the order of $\frac{K_BT}{E_F} = f_{thermal}$ ②

∴ For every electron the rise in energy is $\Delta E = \cancel{K_BT}\ \epsilon_{thermal} \cdot f_{thermal}$

$$= K_BT \cdot \left(\frac{K_BT}{E_F}\right)$$

Energy rise for N_A electrons is

$$\Delta E = N_A \Delta \epsilon$$

$$= K_B N_A \frac{K_B T^2}{E_F}$$

$$= R \frac{K_B T^2}{E_F}$$

$$\therefore C = \frac{d.\Delta E}{dT}$$

$$= 2R \frac{K_B T}{E_F}$$

(2) $$= R \cdot 2 \left(\frac{K_B T}{E_F}\right)$$

@ Room temperature

$$\frac{K_B T}{E_F} \sim \frac{0.0259}{3} = \frac{26}{3} \cdot 10^{-3}$$

$$= 7$$

$$\Rightarrow C \simeq 14 \cdot 10^{-3} R$$

$$= 0.01 R$$

4. Density of states **[10 M]**

a) What is the meaning of density of states function? What is its SI unit? [BT 1][2 M]

b) If the density of states of a material is a constant $Z(E) = k$ and the electron density is n,
   i. what is the Fermi level at $T = 0K$?
   ii. What is the Fermi level at $T \neq 0K$? [BT 3][4 M]

c) Sketch the density of states function
   i. for the conduction band of an intrinsic semiconductor.
   ii. Repeat part (i) for the valence band. [BT 2][4 M]

④ Density of states

a) What is the meaning of DOS function?
What is its SI unit?

Solution:

Density of states is defined as rate of change of the number of states per unit volume upto energy E with respect to ~~E~~ energy E

$$Z(E) = \frac{d\left(\frac{N}{V}\right)}{dE}$$ (1)

where N = total number of states upto energy E

V = volume of material

S I units are

$$[Z] = \left[\frac{\frac{N}{V}}{E}\right] = \left[\frac{N}{EV}\right]$$

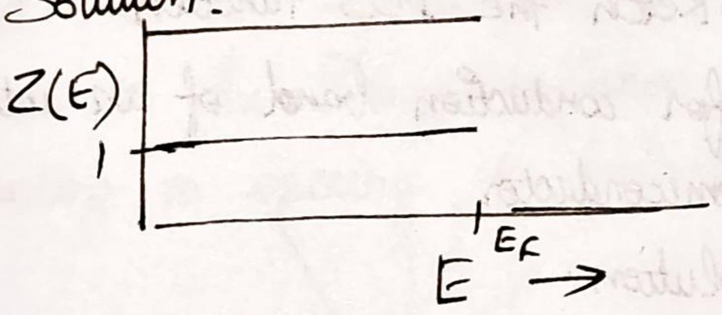
If material is 3D,
then SI unit is $J^{-1}m^{-3}$.

If material is 2D,
then SI unit is $J^{-1}m^{-2}$. (1)

(b) If the DOS of material is a constant $Z(E) = k$ and electron density is n,

(i) what is E_F at $T = 0K$?

Solution:



So @ T=0K, below E_F, all levels are occupied

$$\therefore n = \int_0^{E_F} Z(E)\, \cancel{dE}\, dE$$

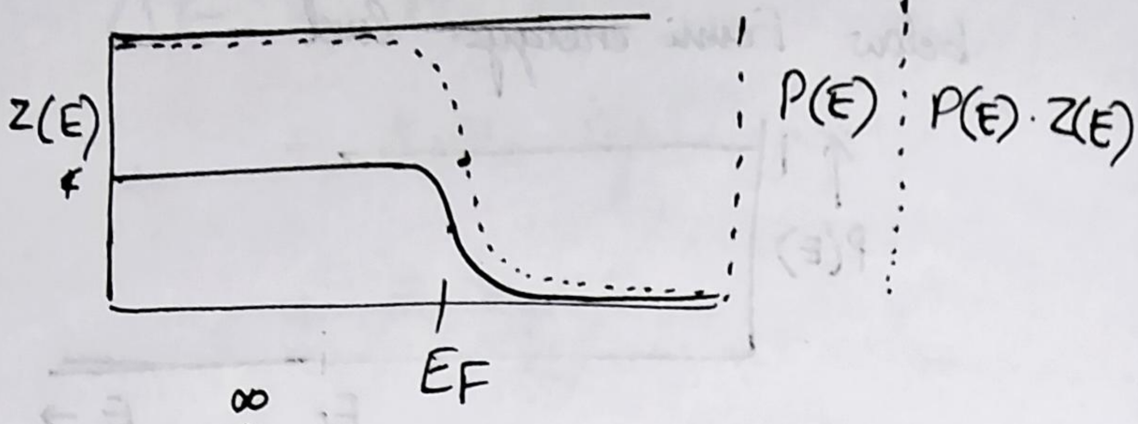
and Z is a constant

$$n = k\int_0^{E_F} dE = kE_F$$

$$\therefore E_F = \frac{n}{k}$$ (2)

(ii) What is the Fermi level at $T \neq 0K$?

Solution :



$$n = \int_0^\infty Z(E)\, P(E)\, dE$$

$$= K \int_0^\infty \frac{1}{1+\exp\left(\frac{E-E_F}{K_B T}\right)}\, dE$$

Now due to symmetry of FD about E_F, the electron at energy ΔE to the left occupies energy level ΔE to the right.

(2) This results in no change in E_F.

$$\therefore \quad E_F = \frac{n}{K}$$

✪ ⓒ part in next page

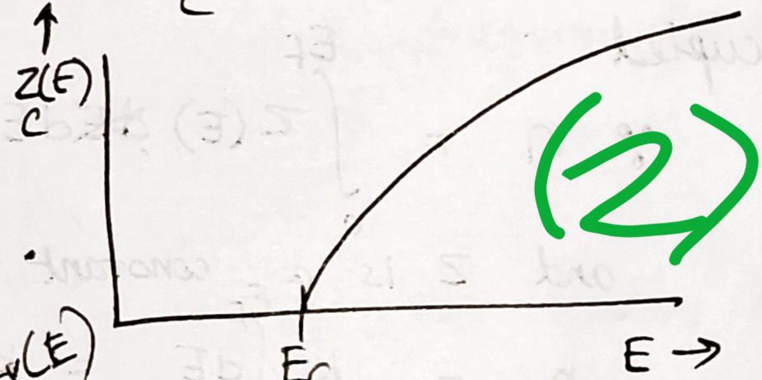
Continued for ④ from previous page

✪ ④ (C) Sketch the DOS function

(i) for conduction band of an intrinsic semiconductor

Solution:

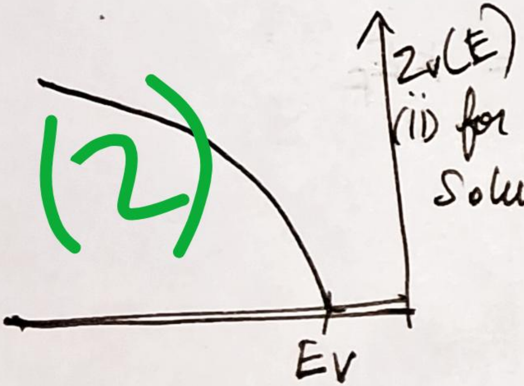
$$Z_C(E) \propto \sqrt{E-E_C}$$



(2)

(ii) for valence band ~~of~~

Solution: $Z_V(E) \propto \sqrt{E_V-E}$



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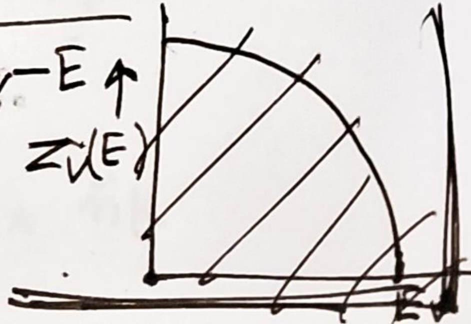


5. E-k diagram [10 M]

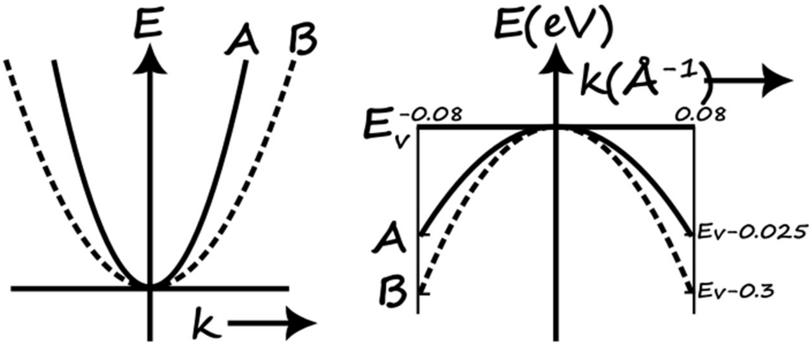
a) Sketch the E vs k diagram for a free electron. [BT 1][1 M]

b) Sketch the E vs k diagram for an electron in a periodic potential. [BT 1][1 M]

c) Consider an intrinsic semiconductor with all electrons occupying states in the lowest valence band at $T = 0K$. Plot the E vs k showing occupancy of levels at both $T = 0K$ and $T \neq 0K$. [BT 2][2 M]

d) Two possible conduction bands are shown in the E vs k diagram given in Figure. 1(a). State which band will result in the heavier electron effective mass; state why [BT 2][2 M]

e) Figure. 1(b) shows the parabolic E vs k relationship in the valence band for a hole in two particular semiconductor materials. Determine the effective mass (in units of the free electron mass) of the two holes. [BT 3][4 M]



(a) (b)

Figure 1: (a) Conduction and (b) valence bands of materials A and B.

⑤ E-K diagram

a) Sketch the E vs K diagram for a free electron.

Solution:

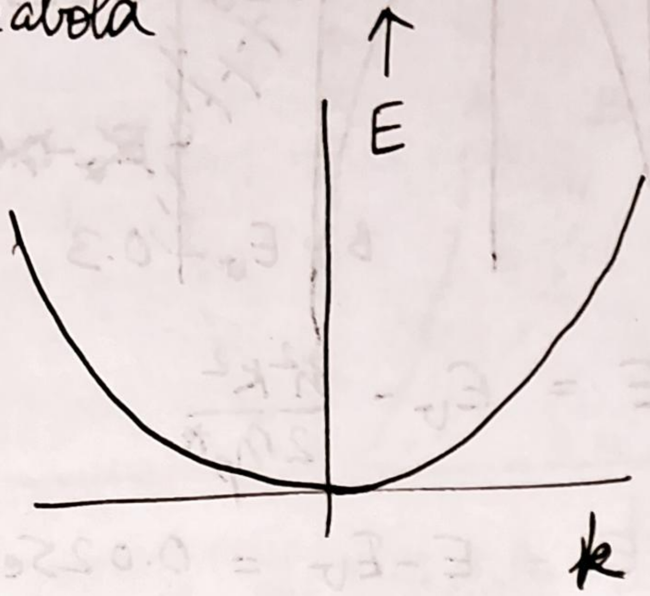
For a free electron, the relation between energy E & momentum p is given by

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

but $p = \frac{h}{\lambda} = \frac{h}{2\pi}K = \hbar K$.

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

So the E vs k diagram will look like a parabola

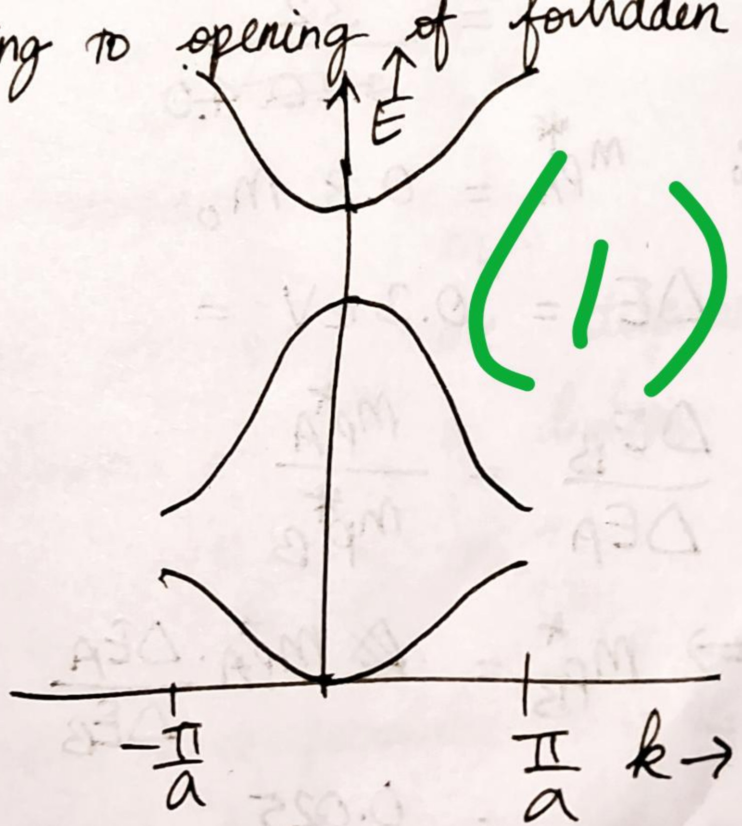


(1)

b) Sketch the E vs k diagram for an electron in a periodic potential.

Solution:

Due to the periodic potential, the band diagram folds at Bragg reflection points and due to hybridization, the degenerate levels at the Bragg reflection points split leading to opening of forbidden levels.



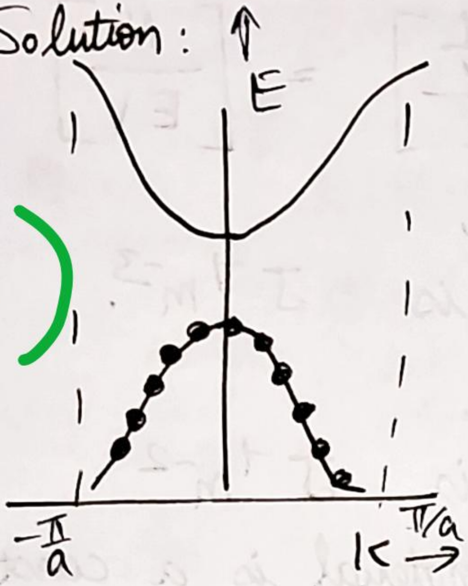
(1)

If periodicity of potential is a, then the Bragg reflection points are $\pm \frac{\pi}{a}$

c) Consider an intrinsic semiconductor with all electrons occupying states in the lowest valence band at T = 0 K. Plot the E vs k diagram showing occupancy of levels at both T = 0 K and T ≠ 0 K.

Solution:

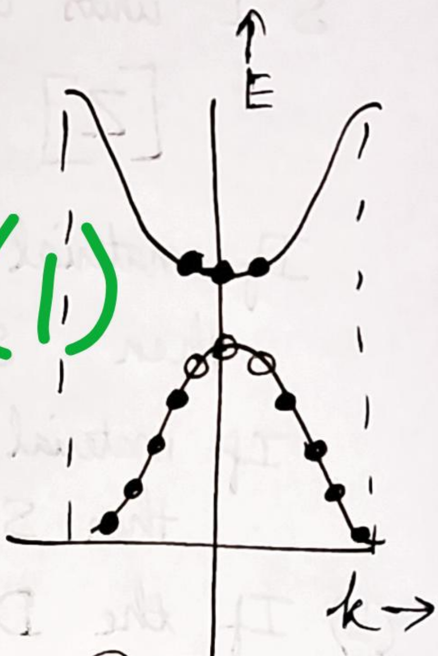
(1)



@ T = 0 K

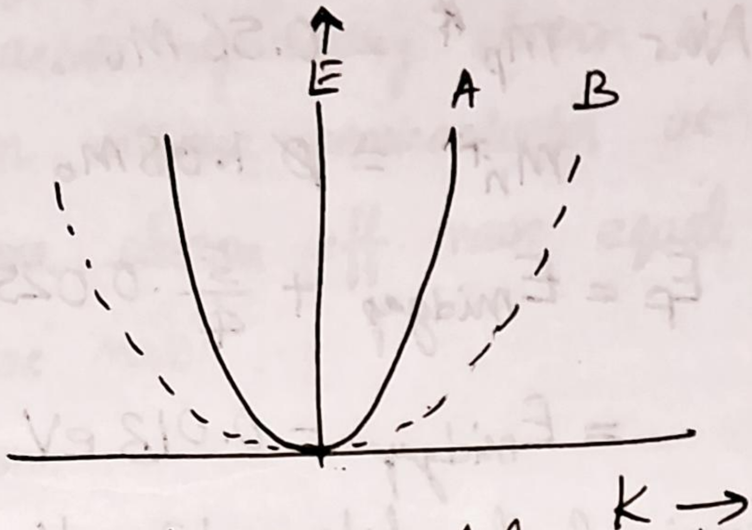
vs

(1)



@ T ≠ 0K

(d) Two possible conduction bands are shown in the E vs k diagram. State which band will result in heavier electron effective mass; state why?



The E vs k for parabolic conduction bands is given by

$$E = \frac{\hbar^2 k^2}{2 m_n^*}$$

The steepness of parabola is given by its double derivative

$$\frac{dE}{dk} = \frac{\hbar^2}{2 m_n^*} 2k = \frac{\hbar^2 k}{m_n^*}$$

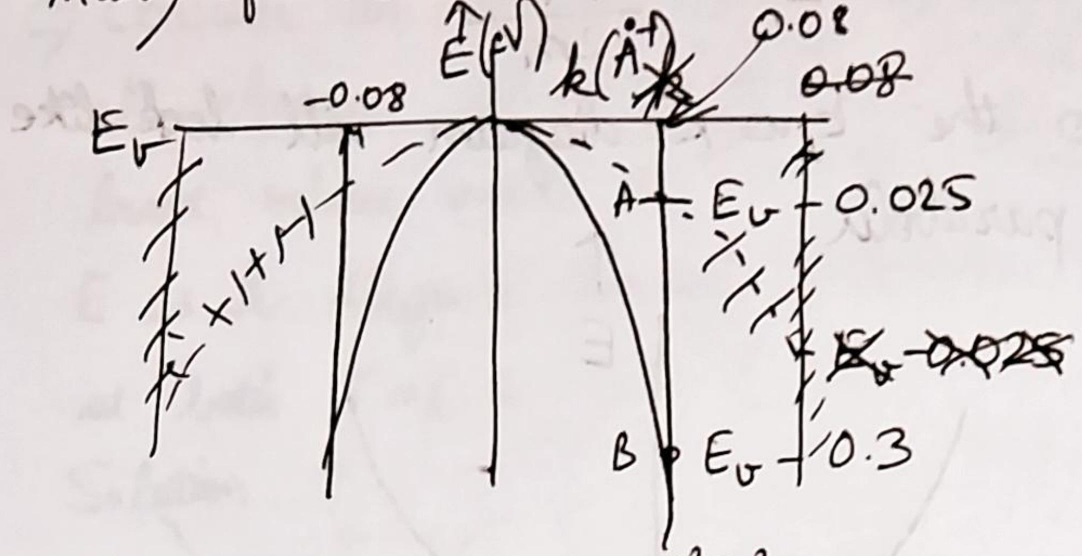
$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m_n^*} \quad (1)$$

So steepness $\propto \frac{1}{m_n^*}$

Since A has more steepness than B, electron in A is lighter than in B.

$\therefore \; m^*_{n_B} > m^*_{n_A}$. (1)

(e) Figure shows parabolic E vs k relationship in valence band for a hole in two materials. Determine the effective mass (in units of free electron mass) of the two holes.



Now $E = E_v - \frac{\hbar^2 k^2}{2 m_p^*}$ (2)

For A, $\Delta E = E - E_v = 0.025\,eV = \frac{\hbar^2 (0.08\,Å^{-1})^2}{2 \cdot m_{p_A}^*}$

$$\Rightarrow m_{p_A}^* \simeq \frac{(10^{-34})^2 \cdot (0.08 \cdot 10^{10})^2}{2 \cdot 0.025 \cdot 1.6 \cdot 10^{-19}}$$

$$\Rightarrow \frac{m_{p_A}^*}{m_0} = \frac{10^{-68} \cdot 64 \cdot 10^{16}}{2 \cdot 9.1 \cdot 10^{-31} \cdot 2.5 \cdot 10^{-2} \cdot 1.6 \cdot 10^{-19}}$$

$$\simeq \frac{3.2 \cdot 10^{-52}}{10^{-31} \cdot 2.5 \cdot 1.6 \cdot 10^{-21}}$$

$$= \frac{3.2}{\cancel{3.20}\ 4.0}$$

$$\begin{array}{r} 1.6 \\ \times 2.5 \\ \hline 4.00 \end{array}$$

$\therefore m_{p_A}^* = 0.8\, m_0$ (1)

For B, $\Delta E = 0.3\,eV =$

$$\frac{\Delta E_B}{\Delta E_A} = \frac{m_{p_A}^*}{m_{p_B}^*}$$

$$\Rightarrow m_{p_B}^* = m_{p_A}^* \cdot \frac{\Delta E_A}{\Delta E_B}$$ (1)

$$= \frac{0.025}{0.3}\, 0.8\, m_0$$

$$= \frac{0.02}{0.3}\, m_0 = \frac{0.2}{3}\, m_0 = 0.06\, m_0$$

6. Fermi level in semiconductors **[10 M]**

a) Sketch the energy band diagram showing the density of states, Fermi-Dirac probability function and areas representing electron and hole concentration for an intrinsic semiconductor at $T \neq 0K$. Assume electron effective mass is equal to hole effective mass. [BT 1, 2][3 M]

b) Calculate position of Fermi level with respect to center of the bandgap in silicon for
   - i. $T = 0\ K$, and
   - ii. $T = 300\ K$.

   The electron effective mass is $1.08m_0$ and hole effective mass is $0.56m_0$. [BT 2][2 M]

c) Draw, compare, and contrast the sketches of the energy band diagram for p-type semiconductor at $T = 0K$ and $T = 300K$. [BT 3][2 M]

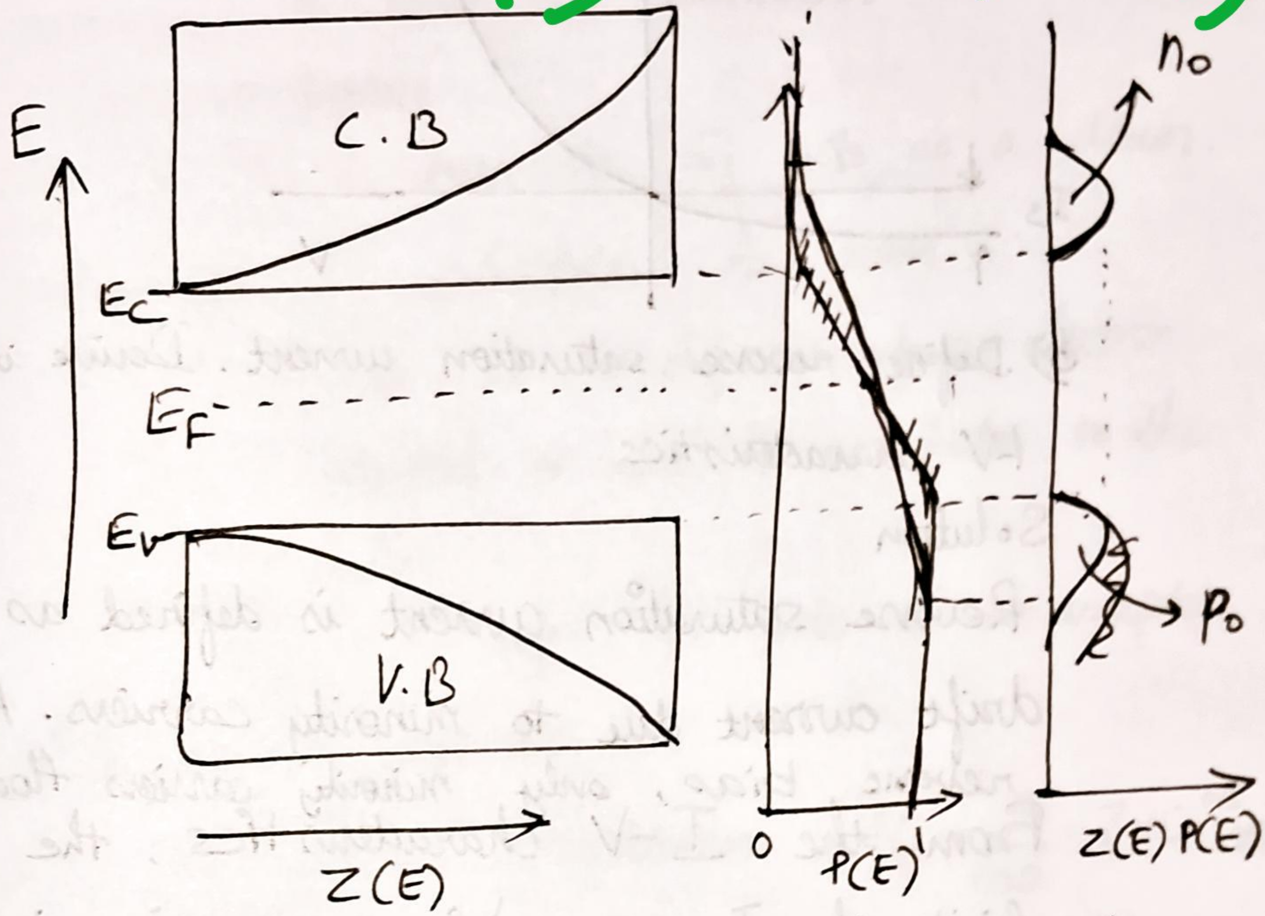
d) Silicon atoms, at a concentration of $7 \cdot 10^{15} cm^{-3}$, are added to GaAs. Assume that the silicon atoms act as fully ionized dopant atoms and that 5% of the dopants replace Ga atoms and 95% replace As atoms.
   - i. Determine the donor and acceptor concentrations.
   - ii. Is the material n type or p type? [BT 2][3 M]

⑥ Fermi level in semiconductors

a) Sketch the energy band diagram showing density of states, Fermi-Dirac probability distribution and areas representing electron and hole concentration for an intrinsic semiconductor at $T \neq 0K$. Assume electron eff. mass equal to hole effective mass.

Solution:

(1) (1) (1)



b) Calculate position of Fermi level with respect to center of band gap in silicon for

(i) $T = 0K$

$$E_F = E_{midgap} + \frac{3}{4} K_B T \ln \frac{m_p^*}{m_n^*}$$ (1)

@ $T = 0K$, correction term is zero

$$\therefore E_F = E_{midgap}$$

(ii) $T = 300K$

$$E_F = E_{midgap} + \frac{3}{4} k_B T_{300} \ln \frac{m_p^*}{m_n^*}$$

Now $m_p^* = 0.56 M_0$

$m_n^* = \cancel{0}\, 1.08 M_0$

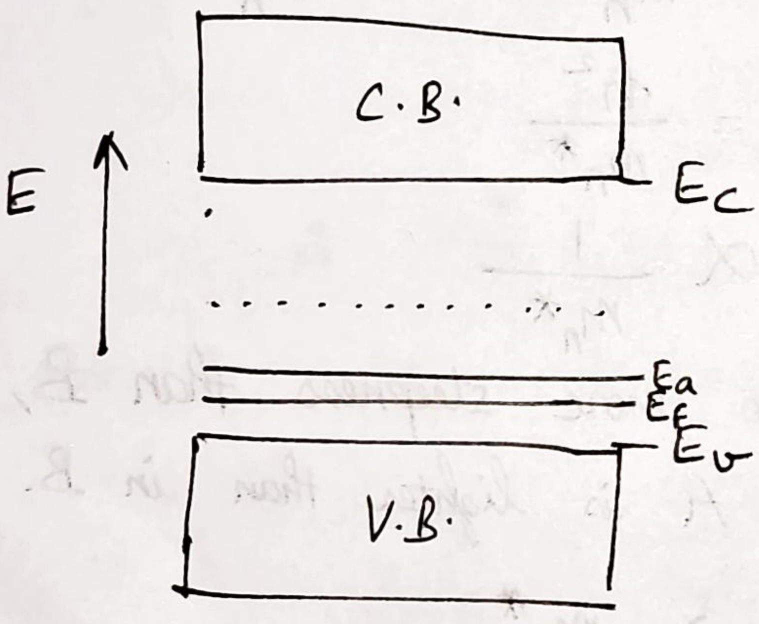
$$\therefore E_F = E_{midgap} + \frac{3}{4} \cdot 0.0259 \ln\left(\frac{0.56}{1.08}\right)$$

$$= E_{midgap} - 0.013 \text{ eV}$$ (1)

So, Fermi level shifts 13 meV below midgap level.

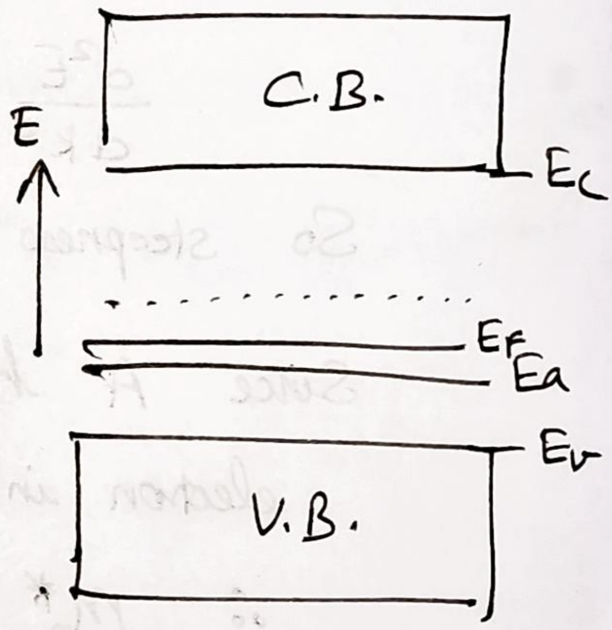
c) Draw, compare, and contrast the sketches of the energy band diagram for p-type semiconductor at T = 0 K and T = 300K.

Solution :



@ T=0K

(1)



@ T=300K

(1)

d) Silicon atoms, at a concentration of $7\cdot10^{15}\,cm^{-3}$ are added to GaAs. Assume that silicon atoms are fully ionized and that 5% of dopants replace Ga atoms and 95% replace As atoms.

(i) Determine the donor and acceptor concentrations

Solution

Case (α) Silicon replaces Ga atom

then Si provides an electron additional to what Ga contributes to the lattice.

(1)

Therefore Si acts as a donor.

Case (β) Si substitutes As atom

then Si is deficient of an electron compared to what As contributes to the lattice.

Therefore Si acts as an acceptor.

5% of Si replaces Ga

(1)

$$\Rightarrow \text{Donor concentration} = N_d = \frac{5}{100}\cdot 7\cdot10^{+15}\,cm^{-3}$$

$$= 3.5\cdot10^{+14}\,cm^{-3}$$

95% of Si replaces As

$$\Rightarrow \text{Acceptor concentration} = N_a = (70 - 3.5)10^{14}$$

$$= 6.65\cdot10^{15}\,cm^{-3}$$

(ii) Is the material n type or p type?

Solution: Since $N_a > N_d$, material is p-type (1)

7. p-n junction diode **[10 M]**

a) Write the equation and sketch the $I - V$ characteristics of pn junction diode. [BT 1][2 M]

b) Define reverse saturation current of pn junction diode. Derive it from the $I - V$ characteristics. [BT 1][2 M]

c) A silicon diode can be used to measure temperature by operating the diode at a fixed forward-bias current. The forward bias voltage is then a function of temperature. Assume that the reverse saturation current is proportional to exp $(-E_g/k_BT)$. At $T = 300K$, the diode voltage is found to be $0.60V$. Determine the diode voltage at $T = 310K$. What is the percentage change in voltage? [BT 4][3 M]

d) The pn junction diode can also be used as a temperature sensor by operating the diode at a fixed reverse-bias voltage. What is the percentage change in current for the same temperature rise? [BT 4][2 M]

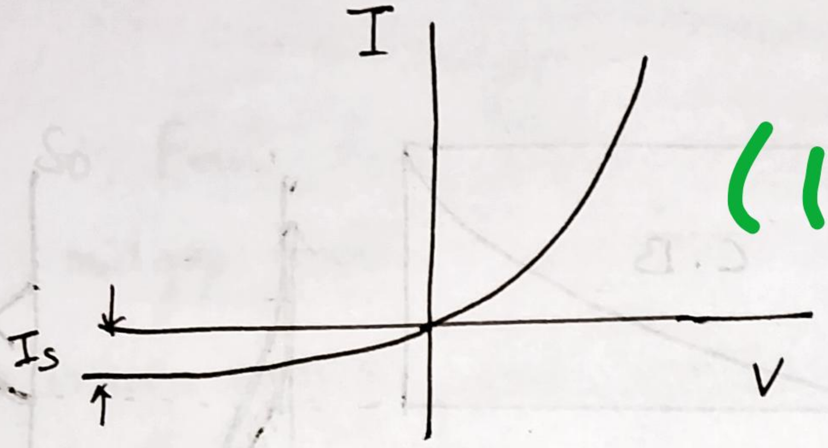
e) Which mode is more sensitive, the constant forward current mode or constant reverse voltage mode? [BT 2][1 M]

⑦ p-n junction diode

a) Write the equation and sketch the I-V characteristics of pn junction diode.

Solution:

(1) $$I = I_s\left[\exp\left(\frac{eV}{k_BT}\right) - 1\right]$$



b) Define reverse saturation current. Derive it from I-V characteristics.

Solution

(1) Reverse saturation current is defined as the drift current due to minority carriers. At high reverse bias, only minority carriers flow. From the I-V characteristics, the limit of I as $V \to -\infty$ is given by

$$\underset{V\to-\infty}{\mathrm{Lt}}\ I = \underset{V\to\infty}{\mathrm{Lt}}\ I_s\left[\exp\left(\frac{-\infty}{k_BT}\right) - 1\right]$$

$$= \underset{V\to-\infty}{\mathrm{Lt}}\ I_s\left[0 - 1\right]$$

$$= -I_s$$ (1)

c) A silicon diode can be used to measure temperature by operating the diode @ a fixed forward bias current. The forward bias voltage is then a function of temperature. Assume that the reverse saturation current is proportional to $\exp\left(-\frac{E_g}{K_BT}\right)$. At $T = 300K$, the diode voltage is found to be 0.60V. Determine the diode voltage at $T = 310K$. What is the percentage change in voltage?

Solution:

Diode operating at constant forward bias current.

The diode I-V characteristic is

$$I = I_S\left[\exp\left(\frac{eV}{K_BT}\right) - 1\right]$$

∴ @ forward bias

$$\exp\left(\frac{eV}{K_BT}\right) \gg 1$$

$$\Rightarrow \quad I \simeq I_S \exp\left(\frac{eV}{K_BT}\right)$$

It is given that reverse saturation current is proportional to $\exp\left(-\frac{E_g}{K_BT}\right)$

$$\Rightarrow \quad I_S = I_0 \exp\left(-\frac{E_g}{K_BT}\right)$$

$$\therefore \quad I = I_0 \exp\left(\frac{-E_g}{K_BT}\right)\exp\left(\frac{eV}{K_BT}\right) \quad (1)$$

Now @ $T = 300K$, $V_{300K} = 0.60V$

$$\Rightarrow I = I_0 \exp\left(-\frac{E_g}{k_B T_{300K}}\right) \exp\left(\frac{eV_{300K}}{k_B T_{300K}}\right) \text{ — Ⓐ}$$

and @ $T = 310K$ $V_{310K} = ?$

$$I = I_0 \exp\left(-\frac{E_g}{k_B T_{310K}}\right) \exp\left(\frac{eV_{310K}}{k_B T_{310K}}\right) \text{ — Ⓑ}$$

Ⓑ ÷ Ⓐ gives

$$\exp\left[\frac{eV_{310K}}{k_B T_{310K}} - \frac{eV_{300K}}{k_B T_{300K}}\right] \cancel{\exp} = \exp\left[\frac{E_g}{k_B T_{310K}} - \frac{E_g}{k_B T_{300K}}\right]$$

Taking ln abs.

$$\frac{eV_{310K}}{0.0259 \cdot \frac{310}{300}} - \frac{eV_{300K}}{0.0259} = E_g\left[\frac{1}{0.0259 \cdot \frac{310}{300}} - \frac{1}{0.0259}\right]$$

$$\Rightarrow e\left[V_{310K} \cdot 37.36 - 0.6 \cdot 38.61\right] = E_g\left[37.36 - 38.61\right]$$

Now E_g of Si = 1.12eV

$$\Rightarrow V_{310K} \cdot 37.36 - 23.16 = -1.12 \times 1.25$$
$$= -1.4$$

$$\Rightarrow V_{310K} = \frac{23.16 - 1.4}{37.36}$$

$V_{310K} = 0.58\,V$ (2.5)

$\therefore$ % change in voltage $= \frac{V_{310K} - V_{300K}}{V_{300K}} \times 100$

$= \frac{0.58 - 0.60}{0.60} \times 100$

(0.5)

$= 2.9\%$

d) pn junction diode can also be used as temperature sensor by operating the diode at a fixed reverse bias voltage. What is the percentage change in current for same temperature rise?

Solution: Diode operating at constant reverse bias voltage.

$$I = I_s\left[\exp\left(\frac{eV}{K_BT}\right) - 1\right]$$

~~@T=300K.~~

~~$I = I_s \exp$~~

At sufficient reverse bias

$$I \rightarrow -I_s$$

and $I_s \propto \exp\left(\frac{-E_g}{K_BT}\right)$.

~~$\therefore I_s = I_0 \exp$~~

$$\frac{I_s^{310K}}{I_s^{300K}} = \frac{\exp\left(-\frac{E_g}{K_BT_{310K}}\right)}{\exp\left(-\frac{E_g}{K_BT_{300K}}\right)}$$

(1)

$$\Rightarrow I_s^{310K} = I_s^{300K} \exp\left[-\left(\frac{E_g}{K_BT_{310K}} - \frac{E_g}{K_BT_{300K}}\right)\right]$$

$$\Rightarrow I_S^{310K} = I_S^{300K} \exp\left[-E_g\left(\frac{1}{0.0259\cdot\frac{310}{300}} - \frac{1}{0.0259}\right)\right]$$

$$= I_S^{300K} \exp\left[-\frac{E_g}{0.0259}\left(\frac{300}{310} - 1\right)\right]$$

$$= I_S^{300K} \exp\left[\frac{1.12}{0.0259}\,\frac{10}{310}\right]$$

$$= I_S^{300} \exp\left(1.39\right)$$

$$I_S^{310K} = 4\, I_S^{300K}$$

$$\therefore \%\ \text{change in current} = \frac{I_S^{310K} - I_S^{300K}}{I_S^{300K}} \times 100$$

(1)

$$= \frac{4\, I_S^{300K} - I_S^{300K}}{I_S^{300K}} \times 100$$

$$= 300\,\%$$

(e) Which mode is more sensitive, the constant forward current mode or constant reverse voltage mode?

Solution: constant reverse voltage mode. (1)

8. Solar cell **[10 M]**

a) Sketch the $I - V$ characteristics of pn junction solar cell. [BT 1][1 M]

b) Define short circuit current and open circuit voltage. [BT 1][2 M]

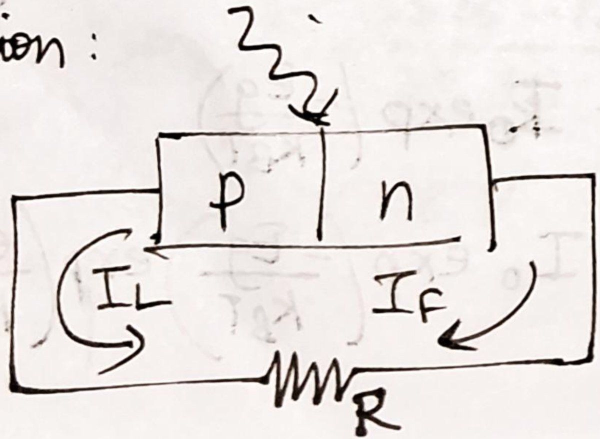
c) A silicon solar cell under standard test conditions has short circuit current density of $35\ mA/cm^2$, and open circuit voltage of $0.60\ V$. The fill factor for the material is 0.80. If the incident power is $100\ mW/cm^2$, calculate the efficiency of the cell. [BT 3][4 M]

d) The energy band gap of a semiconductor is $3\ eV$. Is this material useful for solar cell applications? Give reasons. [BT 4][3 M]

⑧ Solar cell

a) Sketch the I-V characteristics of pn junction solar cell

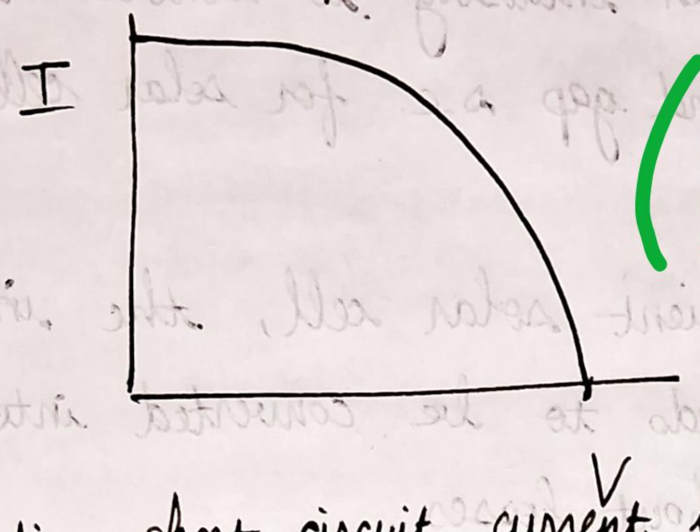
Solution :



$$I = I_L - I_F$$

$$= I_L - I_s\left[\exp\left(\frac{eV}{K_BT}\right) - 1\right]$$

$\therefore$ I - V through load is



(1)

b) Define short circuit current and open circuit voltage

Solution:

(1) Short circuit current is the current generated due to solar cell when the resistance of load is zero.

(1) Open circuit voltage is the voltage generated across the solar cell when the resistance is infinite.

c) A silicon solar cell under standard test conditions has short circuit current density of 35 mA/cm², and open circuit voltage of 0.60V. The fill factor of material is 0.80. If the incident power is 100 mW/cm², calculate efficiency of cell.

$V_{oc} = 0.60V$ $\quad$ $FF = 0.80$

J_{sc} ~~I_{sc}~~ $= 35mA/cm^2$

Input power per unit area $= 100\,mW/cm^2 = I_{in}$

Usable power output per unit area $= V_{oc}\, j_{sc}$

Max power output $=$ Fill factor $\cdot$ Usable power output

(2) $= FF \cdot V_{oc}\, j_{sc}$

So efficiency $= \dfrac{\text{Max power output per unit area}}{\text{Input power per unit area}} \times 100$

$$= \frac{F.F.\, V_{oc} \cdot j_{sc}}{I_n} \times 100$$

$$= \frac{0.8 \cdot 0.60V \cdot 35\, mA/cm^2}{100\, mW/cm^2} \times 100$$

(2) $= 0.48 \cdot 35$

$\simeq 17\%$

d) The energy bandgap of a semiconductor is 3eV. Is this material useful for solar cell applications? Give reasons.

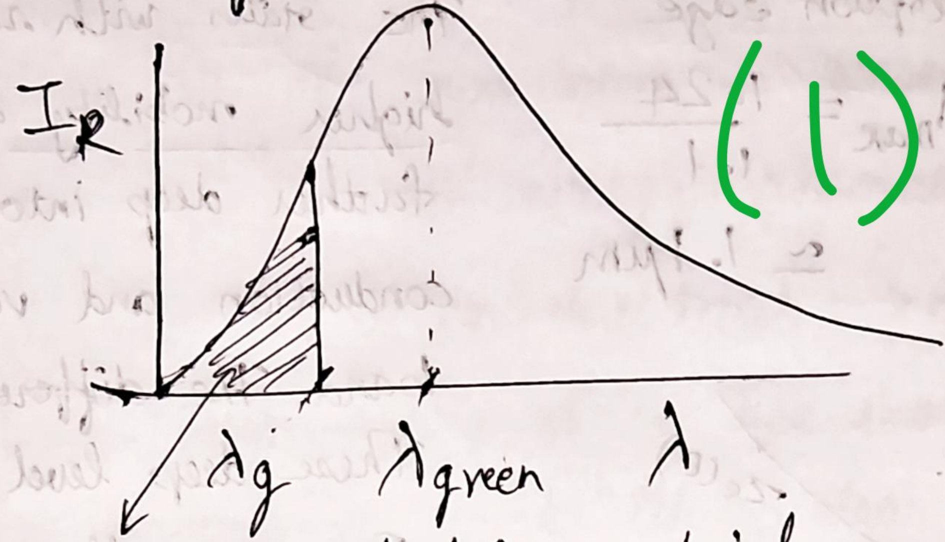
Solution:

· The optical absorption edge for the material is

(1) $(\mu m)\ \lambda_{max} = \dfrac{1.24}{E_g(eV)} = \dfrac{1.24}{3} = 0.41\mu$

So all photons with wavelength less than 0.4 µm are absorbed. However the blackbody radiation spectrum of Sun peaks at $\lambda_{\text{Green}} \simeq 0.51\,\mu m$.

So most of the radiation cannot be absorbed.



(1)

- photons absorbed by material.

- since most of the photons are transmitted, the solar cell is not efficient. (1)

9. Direct and indirect band gap semiconductors **[10 M]**

a) Sketch the $E\ vs\ k$ diagram for
  i. a direct bandgap semiconductor, and
  ii. an indirect bandgap semiconductor.
[BT 1][2 M]

b) Why is direct band gap semiconductor useful for solar cell application? Crystalline silicon is indirect band gap semiconductor. What is the process employed in industry to “convert” it into a direct band gap semiconductor for solar cell application? [BT 2][2 M]

c) Which material is used in blue LED? What is the bandgap of the material? [BT 3][3 M]

d) $Al_xGa_{1-x}As$ is a ternary semiconductor and the energy band gap variation as a function of mole fraction x of $AlAs$ is shown in Figure 1. Which composition can used as material for blue LED application? [BT 4][3 M]

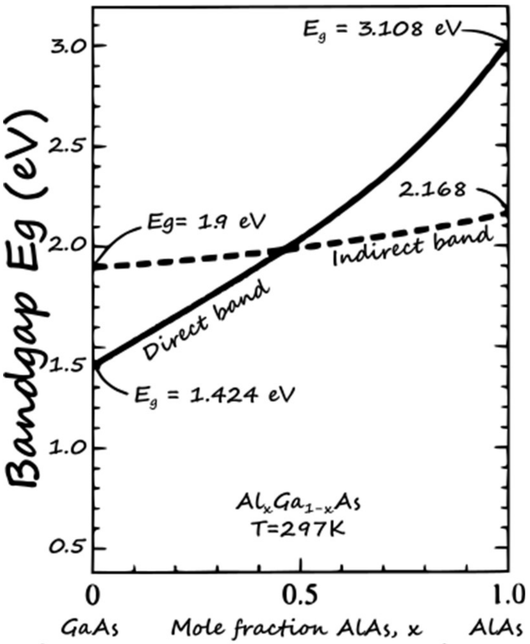
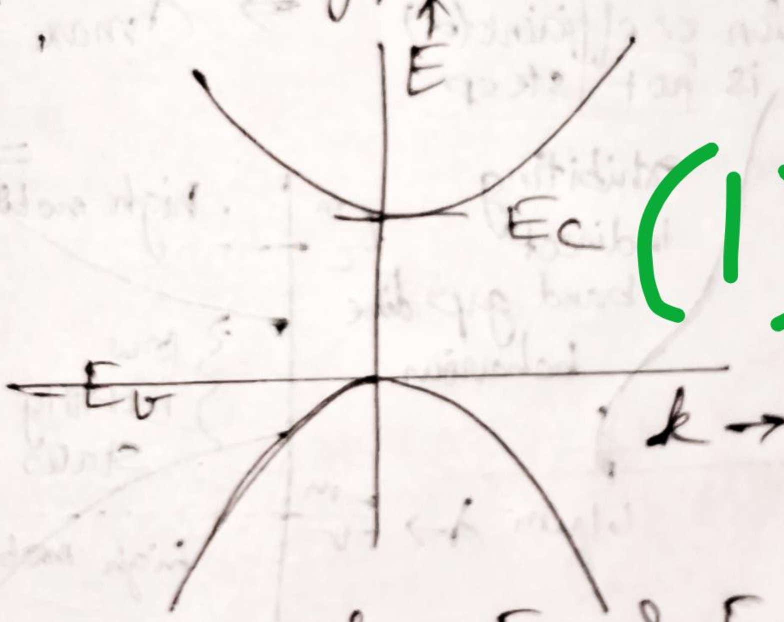


Figure 1. Energy Bandgap

⑨ Direct and indirect band gap semiconductors

a) Sketch the E vs k diagram for

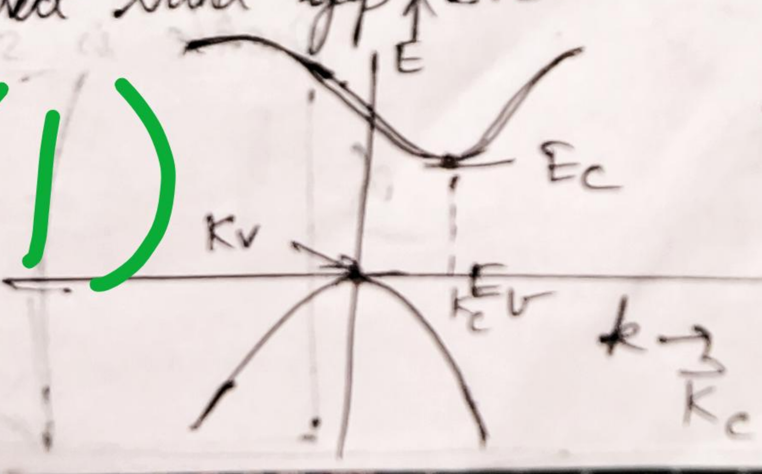
(i) a direct band gap s.c.



(1)

The wavevectors for Ec & Ev are same.

(ii) indirect band gap s.c.



(1)

The wavevectors for E_c & E_V are not same.

$\vec{K}_c - \vec{K}_v = \Delta\vec{K} \neq 0$

b) Why is direct bandgap s.c. useful for solar cell application? Crystalline silicon is indirect band gap s.c. What is the process employed in industry to "convert" it into a direct band gap s.c. for solar cell application?

Solution:

For efficient solar cell, the input optical power needs to be converted into electrical power without losses.

The excess charge carriers at the depletion range ~~are~~ ~~separated~~ generated due to illumination are separated due to the internal electric field.

If the semiconductor is indirect band gap, the optical absorption needs to be accompanied by the absorption of ~~photon~~ phonon.

∴ photon + phonon ⟶ electron + hole

Since the absorption occurs via phonon assistance. Since ~~three~~ four particles are involved (photon, phonon & electron (hole)) the absorption is less efficient. The reason for phonon assistance is to conserve momentum.

However, a direct band gap s.c. does not need assistance from phonon to absorb photon as the momentum is conserved simultaneously with energy conservation

(1) photon + covalent bond → electron-hole

Here only ~~two~~ three particles are involved, so the process is more likely than for indirect s.c.

crystalline-Si was used as early photovoltaic material. However, ~~it~~ since it is an indirect bandgap s.c., the conversion efficiency is low.

When silicon is deposited by Chemical Vapour Deposition (CVD) technique at temperature below 600°C, an amorphous film is formed regardless of type of substrate.

In amorphous Si, there is only very short range order, and no crystalline regions are observed.

4 crystalline Si	amorphous Si
Indirect band gap	like Direct band gap
$E_g = 1.1\,eV$.	Due to short range order, there is no E_g or forbidden band.

. but states with low mobility

The states with relatively higher mobility are further deep into the conduction and valence band. ~~The difference~~ These deep level E_c & E_v are called mobility edges and the difference in energy of these levels is called $\boxed{\text{mobility gap.}}$ The mobility gap is of the order of $\boxed{1.7eV}$

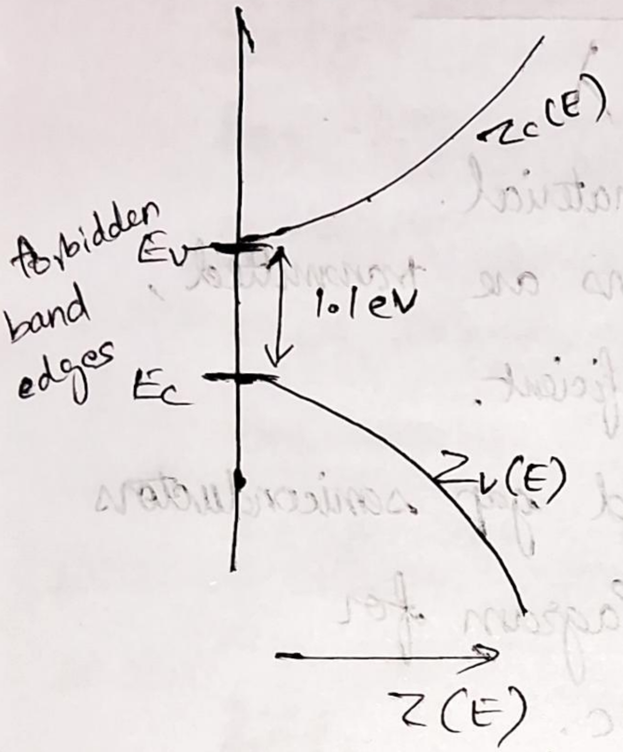
$$\Rightarrow \lambda_{max} = \frac{1.24}{1.7} \mu m$$

$$= 0.73 \mu m$$

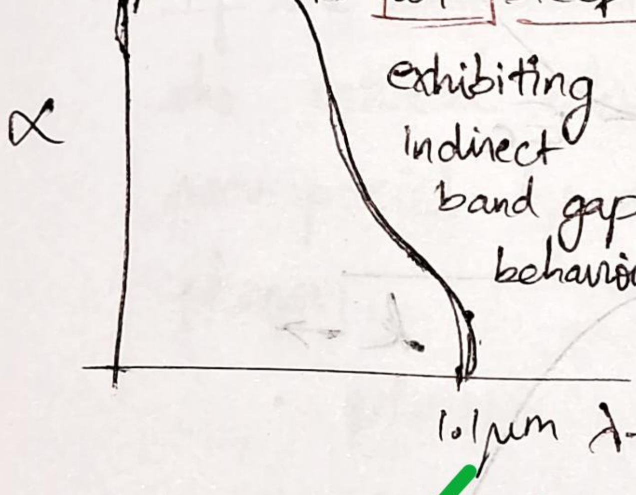
Absorption edge

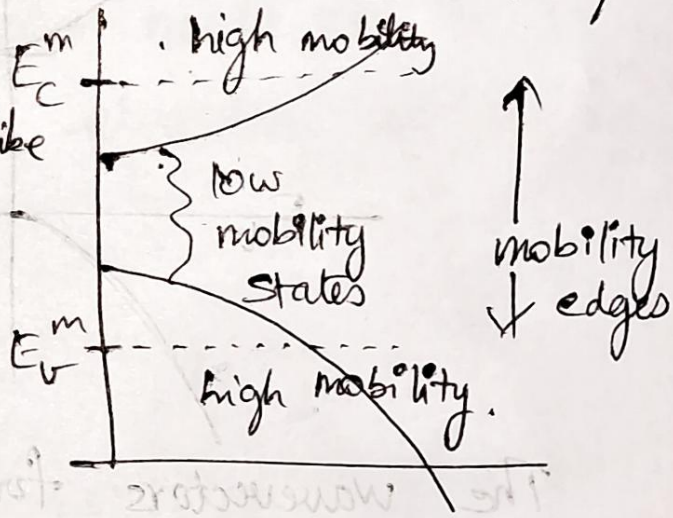
$$@ \lambda_{max} = \frac{1.24}{1.1}$$

$$\simeq 1.1 \mu m$$



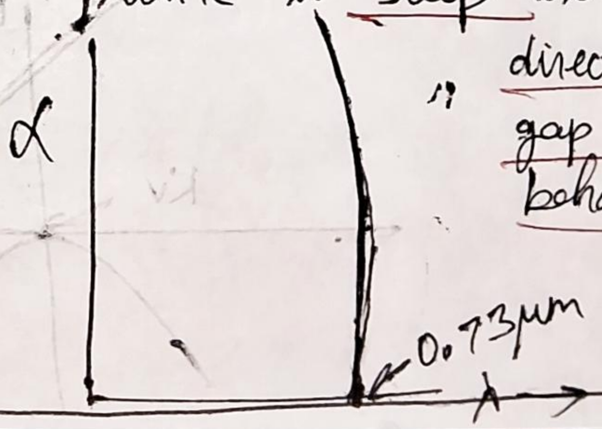
Absorption coefficient(α) profile is not steep


exhibiting indirect band gap like behaviour



(1)

- Absorption coefficient profile is steep exhibiting direct band gap like behaviour.



(C) Which material is used in blue LED? What is the bandgap of material?

Solution: GaN is the base material for blue light emission. (1)

However, it has a direct band gap of 3.4 eV.

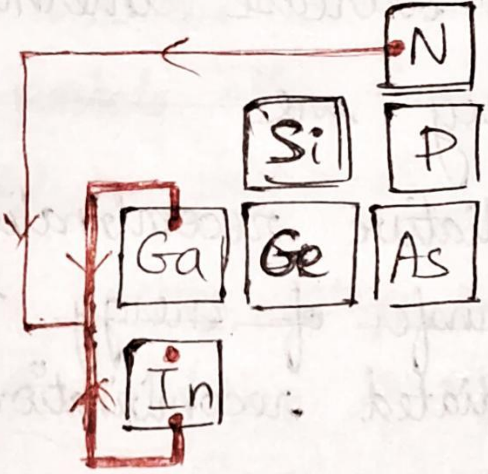
blue photon has 400 nm

So $E_{blue} = \frac{1.24}{0.4} = 3\,eV$ (1)

To reduce the band gap to 3 eV, GaN is alloyed with In to engineer the band gap of blue.

$In_xGa_{1-x}N = x\,InN + (1-x)(GaN)$

This is called band gap engineering.



(1)

(d) Bandgap engineering data for $Al_xGa_{1-x}As$ is given. At what composition blue LED material is formed?

E_g of GaAs = 1.424 eV direct

1 2a

E_g of $x=0.45$ $Al_xGa_{1-x}As$ = 2.0 eV direct the colours possible ~~with~~ are

(1) $\frac{1.24}{1.424}$ μm (1) $\frac{1.24}{\cancel{1.4}2.0}$ μm

$= 0.87$ μm 0.62 μm

620 nm to 870 nm

(1) So Red is possible but not blue (400nm) or green.

10. LED **[10 M]**

a) What are the materials used for red, green, and blue LEDs? [BT 1][2 M]

b) What are the mechanisms that decrease the efficiency of an LED? [BT 1][3 M]

c) The energy band gap variation as a function of mole fraction x of $GaAs_{1-x}P_x$ is shown in Figure 1. What is the range of colours that can be emitted if used for LED application? Report in wavelength. [BT 3][3 M]

d) Calculate the critical angle at GaAs - air interface. The refractive index of GaAs is 3.8 at $\lambda = 0.70\ \mu m$. [BT 3][2 M]

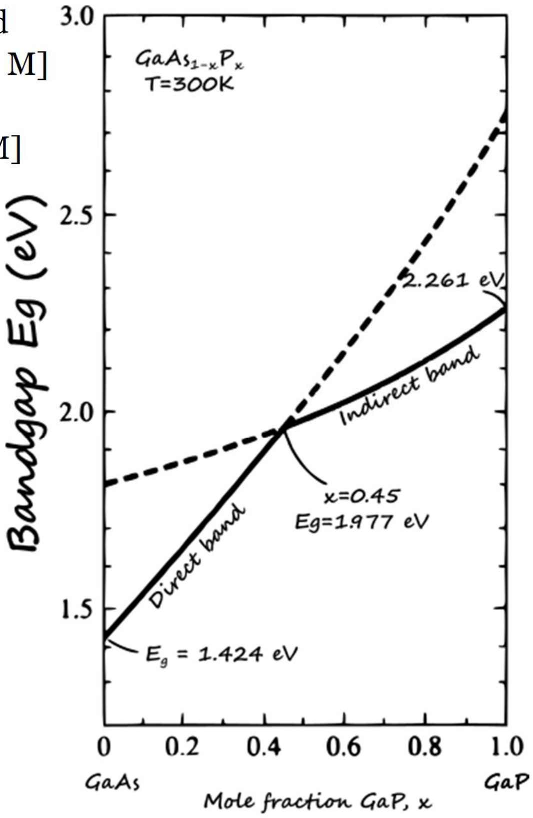


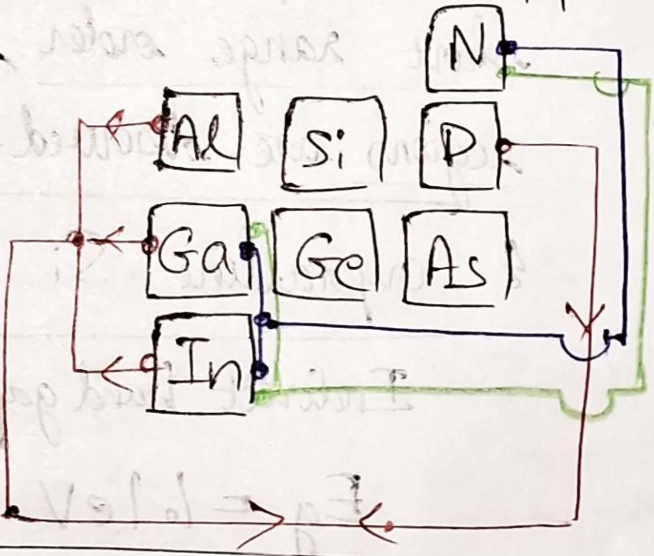
Figure 1. Energy band gap

⑥ LED

a) What are the materials used for red, green and blue LEDs?

Solution

Red	Green	Blue
AlGaInP (modern) high luminous efficiency GaAsP (obsolete) low luminous efficiency	$In_xGa_{1-x}N$ 0.5	1 $In_xGa_{1-x}N$ Nobel prize in Physics 2014



0.5

b) What are the mechanisms that decrease the efficiency of an LED?

Solution:

The luminescent efficiency is defined as the ratio of radiative recombination rate to the ~~non-~~ total ~~radiative~~ recombination rate

$$\eta_q = \frac{R_r}{R}$$

Recombination of excess carriers is of two types.

- Radiative
- Non vadiative

Radiative recombination emits photon

Non radiative recombination transfers energy to particle other than photon - either phonon (heat) or ~~electron~~ other electron or other hole.

Since recombination rate is inversely propotional to the lifetime of the process

$$R \propto \frac{1}{\tau}$$

we can write

$$R = R_r + R_{nr}$$

$$\frac{1}{\tau} = \frac{1}{\tau_r} + \frac{1}{\tau_{nr}}$$

$$\Rightarrow \eta_q = \frac{R_r}{R} = \frac{\frac{1}{\tau_r}}{\frac{1}{\tau_r}+\frac{1}{\tau_{nr}}} = \frac{\tau_{nr}}{\tau_{nr}+\tau_r}$$

To have high efficiency, we need ~~high~~ large non-radiative lifetime so that probability of a non-radiative recombination is small compared to the radiative recombination.

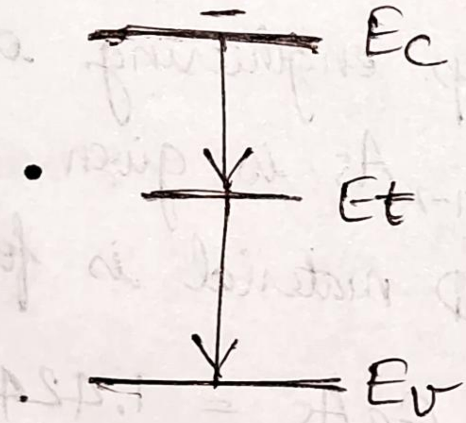
The factors that decide efficiency can be classified as

- internal quantum efficiency
- external quantum efficiency

Internal quantum efficiency is defined as the fraction of diode current that produces luminescence.

The factors that decrease internal quantum efficiency are

- non-radiative recombination events like ~~transfer of energy to trap~~ deep trap-mediated recombination



Deep trap is a defect state that ~~a~~ is away from the band edges and is near the midgap. Due to the ~~high~~ ~~deep~~ ~~lt~~ ~~of~~

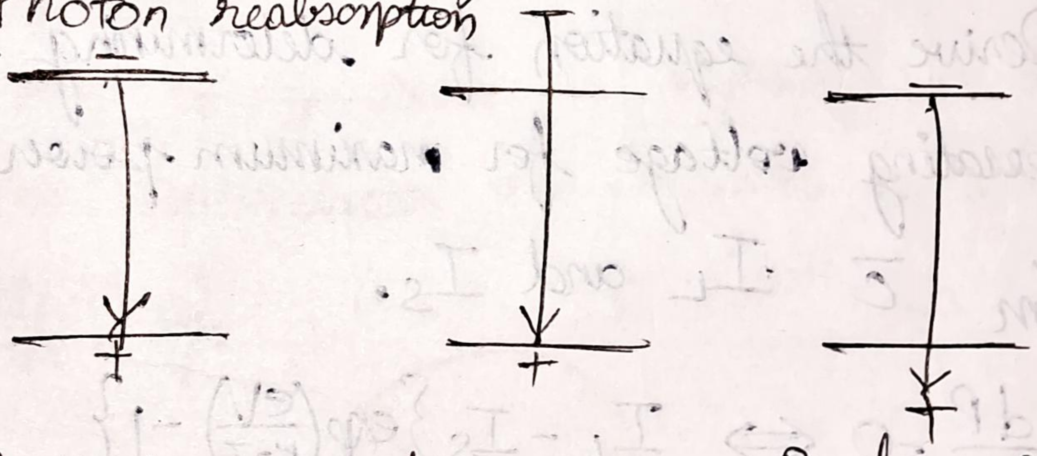
large lifetime of carrier in these states, the electrons get trapped and are unavailable for other ~~recomb~~ radiative recombination processes. If the density of non-radiative trapping sites in the forbidden bandgap increases, the efficiency decreases.

External quantum efficiency refers to the fraction of generated photons that are actually emitted from the semiconductor.

Three mechanisms degrade the external quantum efficiency :-

- Photon reabsorption
- Fresnel loss.
- Critical angle loss.

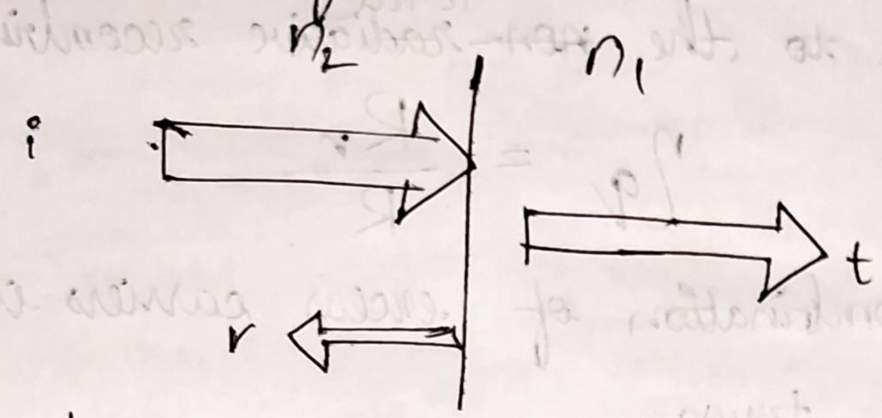
- Photon reabsorption



Radiative recombination can involve energetic electrons ~~and~~ or holes. This can lead to emission of photon with energy greater than band gap.

These energetic photons can be reabsorbed by the material as they satisfy condition optical absorption.

- Fresnel loss
  ~~a~~ Photon generated ~~a~~ must be emitted from semiconductor into air.
  So photon need to transmit across a dielectric interface



If the refractive index of semiconductor is n_2 and air is n_1, then

Reflection coefficient = fraction of light intensity reflected back

$$= \left(\frac{n_2 - n_1}{n_2 + n_1}\right)^2$$

This is called Fresnel loss.

- Critical angle loss.
  Fresnel loss is at normal incidence
  If light is incident at angle > critical angle, it experiences Total Internal Reflection
  So these photons will be reflected back into the semiconductor

(3)

$$\boxed{\theta_c = \sin^{-1}\left(\frac{n_1}{n_2}\right)}$$ Snell's law

c) Energy band gap engineering datta for $GaAs_{1-x}P_x$ is given. What is the range of colours that can be emitted if used for LED application?

(3)

@x=0 1.424 eV to @x=0.45 1.95 eV

$\Rightarrow \lambda = \frac{1.24}{1.424}$ to $\lambda = \frac{1.24}{1.95}$

$= 0.87\,\mu m$ to $\lambda = 0.635\,\mu m$

So 635 nm to 870 nm

d) Calculate critical angle at GaAs-air interface.

$n_{GaAs} = 3.8$ at $\lambda = 0.70\,\mu m$

(2)

$$\theta_c = \sin^{-1}\left(\frac{1}{3.8}\right) = 15.3^\circ$$

So if $\theta_i > \theta_c$, photon will be reflected back into the semiconductor. Hence epoxy resin is deposited on top of the semiconductor to increase external quantum efficiency.