

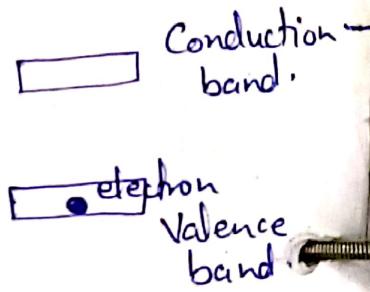
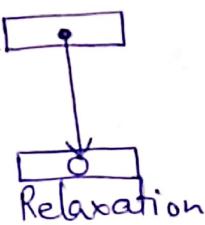
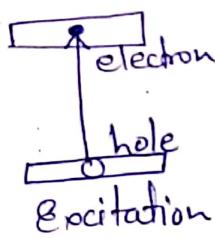
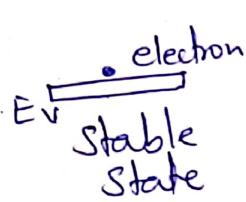
UNIT- III (First topic). (4)

CONCEPTS OF OPTICAL TRANSITION IN BULK SEMICONDUCTOR -

Process in which a atom or molecule changes from one energy state to another state and emits or absorbs electromagnetic radiation in visible, infrared or UV region.

Transitions of e^- from low energy state to high energy states are called Excitations, whereas that from ~~to~~ high energy state to lower energy states are referred to as relaxations.

fig 1- EC



The transition of e^- from high energy state to low energy state in semiconductors are taken as recombination of e^-e^+ pair, that can be radiative and non-radiative emitting photons & phonons respectively.

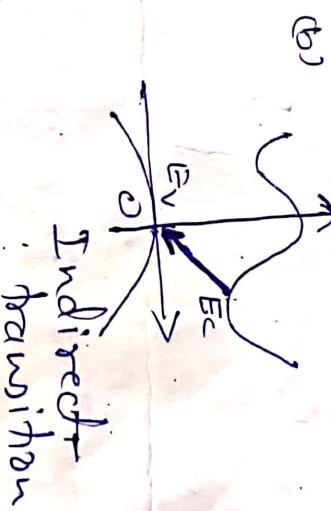
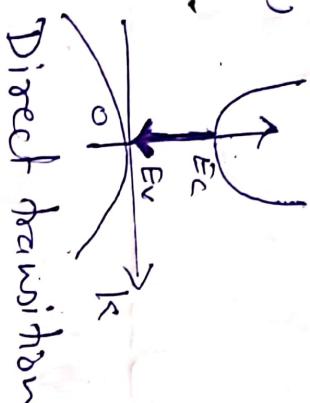
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We can also say that e- are trapped in the defect & transition energy is transformed into forms other than light.

Let us consider the transition

from the bottom of conduction band to the upper of valence band. The semiconductor having such condition for transition placed after common wave vector k , is the direct-transition and that with different k -values is indirect-transition.

fig 2 (a)



Direct transition

Indirect transition

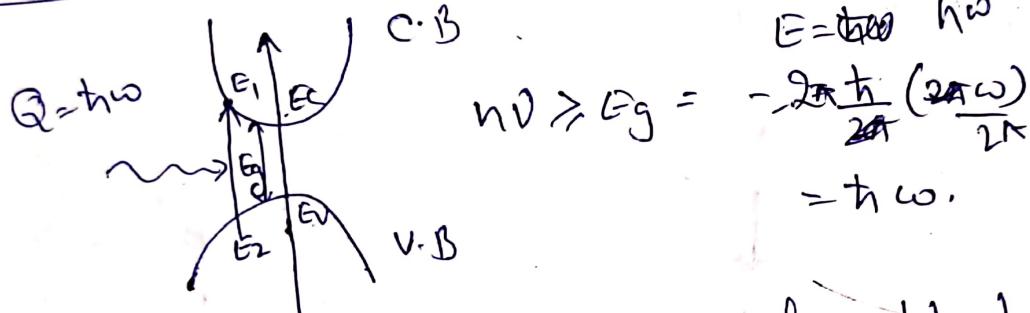
During the transition of electrons, energy & momentum are conserved respectively, so the phonons do not take part in direct transitions, as there wave vector k is much larger than photons. Thus they satisfy the momentum conservation law.

Henceforth, in direct transitions, the transition probabilities are determined only by e- transition probabilities. On the other hand, for indirect transitions, are determined by the

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product of e^- transition probabilities & phonon transition probabilities. This results the direct transition probabilities for direct transition > Indirect transition which gives direct transition semiconductors to be superior than that to the indirect ones for light emitting devices.

OPTICAL ABSORPTION PROCESS



The process takes place when photons with energies greater than band gap energy of semiconductor ($h\nu > E_g$) are absorbed. This gives generation of e^- -hole pair.

e^- -density in C.B is given by

$$E_n = E_c + \frac{\hbar^2 k^2}{2m_h^*}$$

in valence band

$$E_p = E_v - \frac{\hbar^2 k^2}{2m_p^*}$$

$$h\nu = E_n - E_p = E_c - E_v + \frac{\hbar^2 k^2}{2m_h^*} + \frac{\hbar^2 k^2}{2m_p^*}$$

$$\text{or } E_c - E_v + \frac{\hbar^2 k^2}{2} \left(\frac{1}{m_h^*} + \frac{1}{m_p^*} \right) = E_g + \frac{\hbar^2 k^2}{2m_p^*}$$

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where m_r^* = reduced mass.

From this eqⁿ, density of final states have C.B with a parabolic band structure as

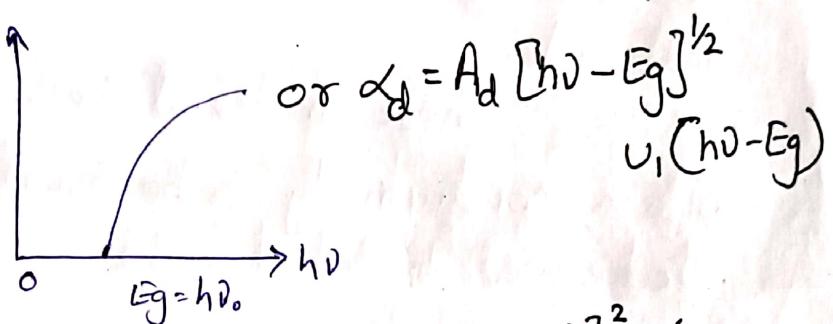
$$g_n(E) = \frac{4\pi}{\hbar^3} (2m_r^*)^{3/2} (\hbar\omega - E_g)^{1/2}$$

$$(\propto \hbar\omega)^2 = A(\hbar\omega - E_g) \quad \xrightarrow{\text{Absorption}}$$

For direct band gap -

$$\alpha_d = A(\hbar\omega - E_g)^{1/2} \quad \Delta k = 0$$

Absorption Coeff. α_d



For Indirect band-gap - $\alpha_i = A_{ph} [\hbar\omega - (E_g - E_{ph})]^2 v_i (\hbar\omega - E_g + E_{ph})$

$$\alpha_i = A'(T) (\hbar\omega - E_g)^2 + A_{ph} [\hbar\omega - (E_g + E_{ph})]^2 v_i (\hbar\omega - E_g - E_{ph})$$

where $A'(T) = \text{Constl. containing parameters}$

pertaining to the bands and temperature.

where $(\propto)^{1/2} = A(\hbar\omega - E_{ph})$ where E_{ph} involves phonons.

EMISSION PROCESS → with all previous basic theory -

Energy in the conduction band is given by

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

where m_e^* = effective mass of e-

Optical Absorption Process -

Ex- For Direct band-to-band absorption, it can take place only at frequencies for which photon energy is $h\nu \geq E_g$ or $\nu = E_g/h$. Corresponding wavelength is $\lambda_c = \frac{hc}{E_g}$ = Band gap wavelength or cut-off wavelength.

During absorption e⁻-hole pair is generated. This increases the mobile charge carrier concentration & increases the conductivity of the material.

These material behaves as photo conductor with a conductivity proportional to photon flux. This effect is used to detect light.

Explanation of Transition rates:—⁽³⁸⁾

From the given figure, consider a light which has a photon energy of $E_{21} = E_2 - E_1$, and a photon density of $n_{ph}(E_{21})$

interacts with a direct-transition semiconductor.

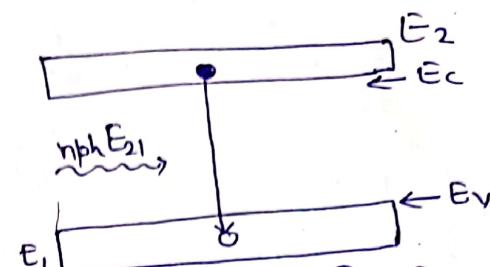


Fig-①

(Model for radiation and absorption).

Under this assumption, we calculate the transition rates for the stimulated emission, the absorption and spontaneous emission. In Fig ① E_c is the energy for the bottom of the conduction band and E_v is the energy for the top of the valence band. This diagram shows the energy bands for a certain ~~and~~ values of K .

- (i) Stimulated Emission Rate:— The stimulated emission rate per unit volume $\tau_{21}(\text{stim})$ is given by a product of the transition probability/time from E_2 to E_1 : B_{21} , the e^- concentration in a state with the energy $E_2: n_2$, the hole concentration in a state with energy $E_1: p_1$, the photon density: $n_{ph}(E_{21})$

The concentration n_2 of the e^- , which occupies a state with energy E_2 in the conduction band, is given as

$$n_2 = p_c (E_2 - E_c) f_2 \quad \text{--- (1)}$$

where $p_c(E_2 - E_c)$ is the density of states, which is a function of $E_2 - E_c$ and f_2 is the distribution function.

The concentration p_1 of a hole, which occupies a state with energy E_1 in the valence band, is given as

$$p_1 = p_v (E_v - E_1) [1 - f_1], \quad \text{--- (2)}$$

where $p_v(E_v - E_1)$ is the density of states, which is a function of $E_v - E_1$, and f_1 = distribution function.

Now, the stimulated emission rate $\tau_{21}(\text{stim})$ is obtained as -

$$\begin{aligned} \tau_{21}(\text{stim}) &= B_{21} n_2 p_1 n_{\text{ph}}(E_{21}) \\ &= B_{21} n_{\text{ph}}(E_{21}) p_c(E_2 - E_c) f_2 p_v(E_v - E_1) (1 - f_1) \end{aligned} \quad \text{--- (3)}$$

(ii) Absorption rate:- The absorption rate / volume $\tau_{12}(\text{abs})$ is given by the product of:-

the transition probability / time from E_1 to E_2 : B_{12}

the concentration of an empty state with energy

E_2 : p_2

the e^- concentration in a state with energy

E_1 : n_1

the photon density : $n_{\text{ph}}(E_{21})$

The concentration p_2 of an empty state, which is not occupied by the e^- with energy E_2 in the conduction

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band is occupied given as

$$\beta_2 = P_c (E_2 - E_c) [1 - f_2] \quad \text{--- (4)}$$

The concentration n_1 of the e^- , which occupies a state with energy E_1 & in the valence band, is given as -

$$n_1 = P_v (E_v - E_1) f_1 \quad \text{--- (5)}$$

Thus, the ~~abs~~ absorption rate $\sigma_{12}(\text{abs})$ is obtained

$$\begin{aligned} \sigma_{12}(\text{abs}) &= B_{12} \beta_2 n_1 n_{\text{ph}}(E_{21}) \\ &= B_{12} n_{\text{ph}}(E_{21}) P_c (E_2 - E_c) [1 - f_2] P_v (E_v - E_1) f_1 \end{aligned} \quad \text{--- (6)}$$

(iii) Spontaneous Emission rate -

Spontaneous Emission rate /volume $\tau_{21}(\text{spont})$ is independent of the incident photon density & is given by the product of -

the transition probability /time from E_2 to E_1 : A_{21} ,

the e^- concentration in a state with energy E_2 : n_2

the hole concentration in a state with energy E_1 : p_1

Using eqn ① & ② ie

$$n_2 = P_c (E_2 - E_c) f_2$$

$$\& P_1 = P_v (E_v - E_1) [1 - f_1]$$

the spontaneous emission rate $\tau_{21}(\text{spont})$ is obtained as

$$\begin{aligned} \tau_{21}(\text{spont}) &= A_{21} n_2 p_1 \\ &= A_{21} P_c (E_2 - E_c) f_2 P_v (E_v - E_1) [1 - f_1] \end{aligned} \quad \text{--- (7)}$$

EINSTEIN'S THEORY OF SPONTANEOUS EMISSION

At thermal equilibrium, the upward transition and downward transition should be equal.

$$B_{12} N_1 Q = A_{21} N_2 + B_{21} N_2 Q \quad \text{--- (1)}$$

$$\text{or } Q = \frac{A_{21}}{\left(\frac{N_1}{N_2}\right) B_{12} - B_{21}} \quad \text{--- (2)}$$

From Boltzmann's distribution law, the ratio of population of two levels, at a given temperature T , is

$$\frac{N_1}{N_2} = e^{(E_2 - E_1)/kT} \quad \text{--- (3)}$$

$$\text{or } \frac{N_1}{N_2} = e^{\hbar\nu/kT} \quad \text{--- (4)}$$

Using eqn (4) in (2) we get

$$Q = \frac{A_{21}}{B_{12} e^{\hbar\nu/kT} - B_{21}} \quad \text{--- (5)}$$

From Planck's black body radiation theory, we have

$$Q = \frac{8\pi hc}{\lambda^5} \frac{1}{(e^{\hbar\nu/kT} - 1)} \quad \text{--- (6)}$$

On equating (5) & (6) we get

$$\frac{A_{21}}{B_{12} e^{\hbar\nu/kT} - B_{21}} = \frac{8\pi hc}{\lambda^5} \frac{1}{(e^{\hbar\nu/kT} - 1)} \quad \text{--- (7)}$$

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$$\text{or } \frac{A_{21}}{B_{21}(e^{h\nu/kT_1})} = \frac{B\pi hc}{\lambda^5(e^{h\nu/kT_1})}$$

γ_2 ~~291~~

(5)

$$\text{or } \left| \frac{A_{21}}{B_{21}} = \frac{B\pi hc}{\lambda^5} \right| \longrightarrow 9$$

Eqn ⑨ gives ratio between spontaneous & stimulated coefficients. A & B are called Einstein's coefficients.

EXPLANATION OF SPONTANEOUS^(u8) EMISSION & STIMULATED EMISSION ①

EMISSION - After absorbing energy, an atom goes to the excited state and does not stay there indefinitely. As a result, there is a transition to ground state E_1 . It is classified as

(i) SPONTANEOUS EMISSION:- This kind of emission does not require any external energy. The atom goes back to its ground state after its lifetime in the excited state. The average lifetime of carriers in the excited state is 10^6 sec. After residing for this much time, they go back to the ground state by emitting energy.

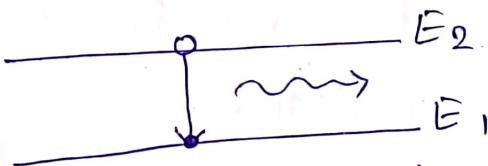


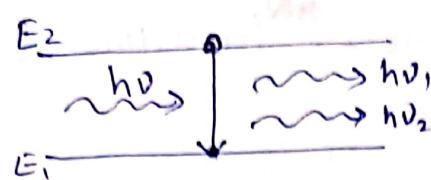
Fig. Spontaneous Emission.

No. of atoms making spontaneous emission / time / volume is given as -

$$N_{sp} = A_{21} N_2 \quad \text{where } A_{21} = \frac{\text{proportionality const}}{\text{const}}$$

N_2 = No. of atoms / volm in the excited state.

(ii) STIMULATED EMISSION:- For this emission, the excited atom is given an external energy and is forced to go to ground state.



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The no. of transitions per unit volume per unit time is given as -

$$N_{st} = B_{21} N_2 Q$$

where B_{21} = constant.

N_2 = No. of atoms per unit volume in the excited state.

Q = Energy density of incident radiation.

(iii) Absorption— The process of raising the atom from the ground state to the excited state is called absorption. Number of atoms per unit volume undergoing absorption is proportional to N_1 , the number of atoms per unit volume in the ground state and Q , the energy density of the incident radiation.

Thus, the number of atoms, undergoing absorption/volume/time is given as

$$N_{ab} = B_{12} N_1 Q$$

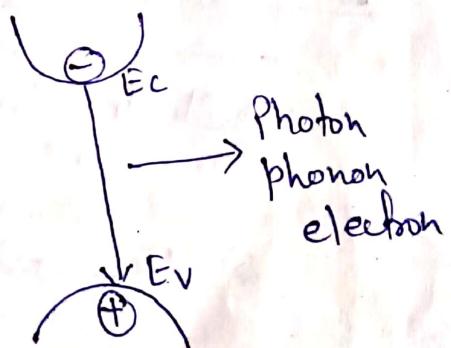
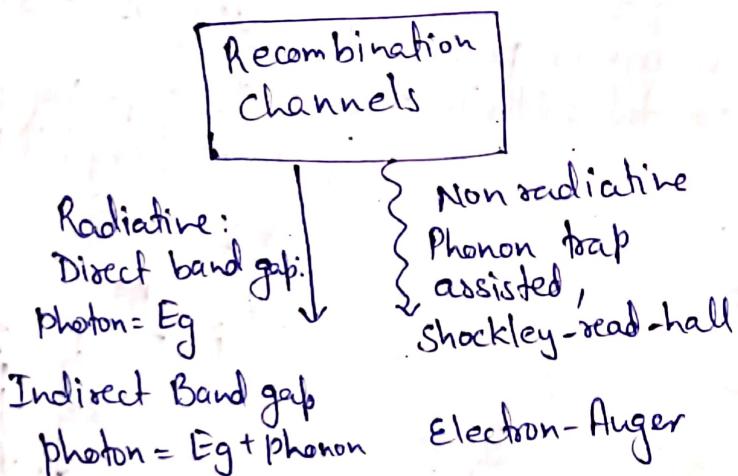
where B_{12} = proportionality constant.

RECOMBINATION PROCESS → With the base of all previous theories -

Till now, we have come to know about the e-hole pair generation. Now we will come to know about the recapturing of e with a hole.

Classification:-

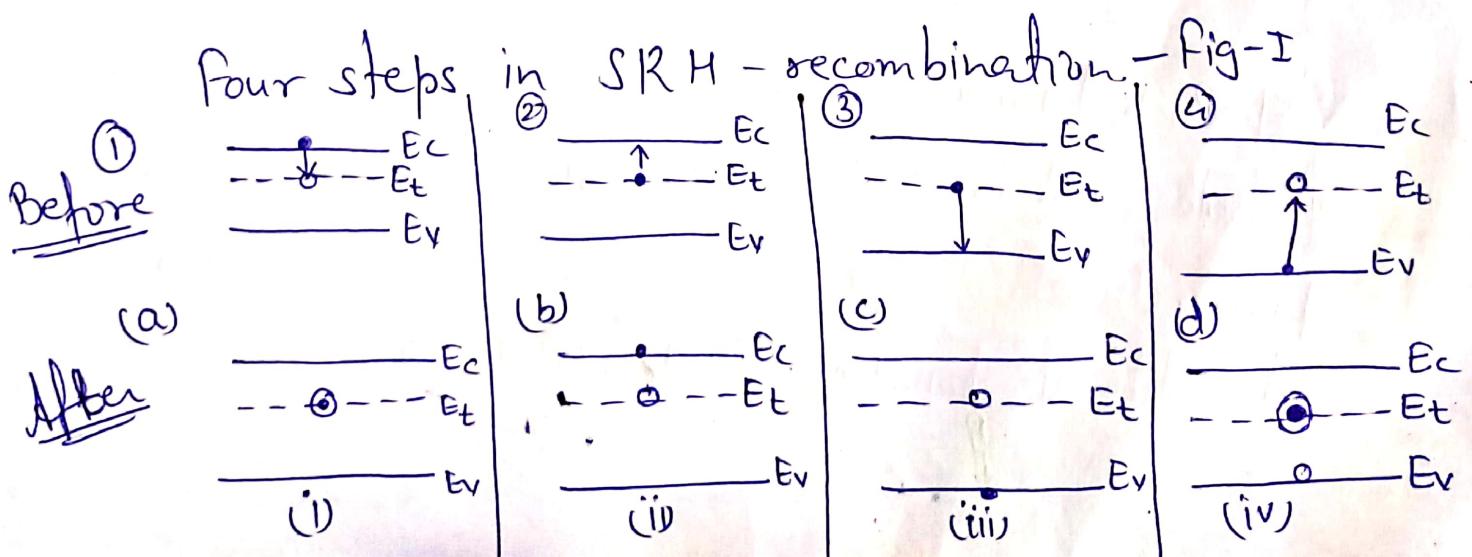
- (i) Band-to-Band recombination giving a photon (radiative)
- (ii) recombination by means of simply giving away energy to the phonons. (SRH-recombination)
- (iii) recombination by transferring kinetic energy to another e- and knocking out into higher energy levels. (Auger recombination)



Shockley - Read - Hall Recombination (SRH)

An indirect recombination process in which the electrons from the lower level of conduction band moves to a defect level (E_t) which is an intermediate or transition level lying between lower level of conduction band (E_c) and higher level of valence band (E_v). This is followed with the photon or phonon emission. From the intermediate level they move to upper level of valence band. It shows that the flaws/defects are essential for this ~~is~~ "SRH recombination".

This recombination process mechanism is named as SRH recombination as it was explained Shockley, Read & Hall. The defects are deep in the crystal structure. Here, we will discuss the single level recombination.



In the fig T, under the before category and after category, the four steps are depicted.

fig (a), (b), (c), (d) are the consequences after the steps of fig 1, 2, 3, 4 are taking place.

In fig (1), see ~~is~~ when the e^- from E_c moves towards E_t which after trapping due to deep level defect, e^- is placed as shown in fig (a). This is step (1).

In second step (ii), e^- from E_t when goes to E_c leaves hole in E_t as shown in fig (b). In step (iii) e^- from E_t may also move to E_V , creating hole in E_t and e^- -hole is annihilated (destroyed) in E_V . In fourth step (iv)

e^- from E_V may also move to E_t creating hole in E_V and e^- will be there in E_t .

Step-1 is named as capturing of e^- . Step-2 is known for emission of e^- . In step-3 capturing of hole and in step-4 emission of hole is taking place. In all the figures, the arrows represents the direction of transition (fig 1, 2, 3, 4)

③

Step (ii) - represents the e^- capture process from E_C to the centre at E_T . In step (iii) there is inverse of emission of e^- from the centre at E_T to the E_C . Step (iv) shows the capturing of hole from the valence band by the centre ~~found in~~ found in E^- . In step (v) the E_T releases out the e^- captured at that point to the valence band (E_V). This step is equal to the process of transferring hole (\circ) from E_V to E_T .

Process (iv), ~~capt~~ shows the capturing of e^- from E_V creating hole in E_V . This process is equivalent to centres (E_T) as if it has ~~been~~ emitted a hole in the valence band (E_V).

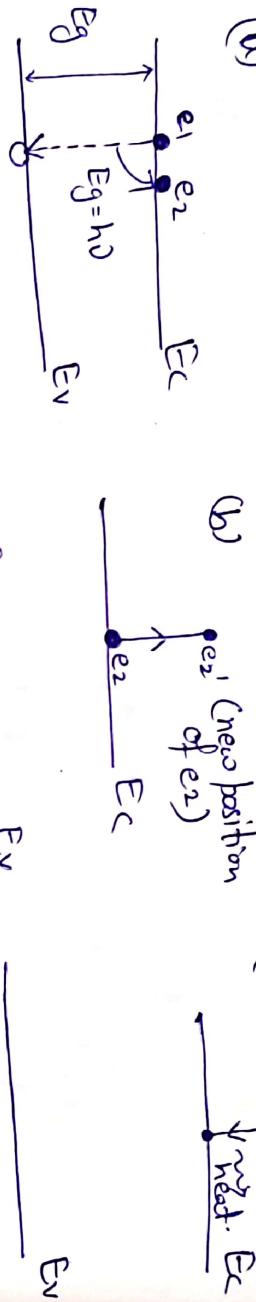
Thus, it is inferred that if E_T is to act as an important recombination centre ~~the~~ must be then ~~process~~ step (i)- e^- capture ~~is~~ followed by step (iv) hole capture and they should have same probability, which will result in going of e^- from E_C to E_V .

On the other hand if e^- capture is step (iv) is followed by step (ii) which is e^- emission the E_T centre acts as e^- trap. Similarly if step (v) is soon followed by step (iv) then the E_T centre is a hole trap. Or else the impurity level will act as recombination centre..



Auger Recombination - Combination with three charge carriers. In this, during the e-hole pair recombination but does not emit photon or phonons, but energy is transferred to the third free e- in the conduction band. The excited e- comes back to the conduction band minimum with the release of energy in the form of heat.

Fig 2 - Auger recombination process (A non-radiative process)



Process is not applicable for light doped materials.

Types -

(I) Direct (Band-to-Band) Auger recombination

(II) Direct (Band-to-Band) Auger recombination
(e-e-h recombination) Two e- and one hole (e-e-h)

process as shown in fig (c)

fig (a) In this one e- in conduction band makes transition to the empty band hole in the valence band. The energy of e-hole pair is transferred to the nearly present e- and

hole in the valence band. The energy of e-hole pair is transferred to the nearly present e- and

(5)

this e^- is excited to ~~at~~ a higher energy level in conduction band. later on, the excited e^- comes back to thermal equilibrium with the emission of its kinetic energy ~~as~~ (lattice phonons). Also possible for ($e-h-h$) in which e^- from conduction band recombines with hole in valence and their recombining energy is given to nearby present hole making it move to lower energy of valence band. Auger recombination is 3rd order process. (eqn contd. from previous notes).

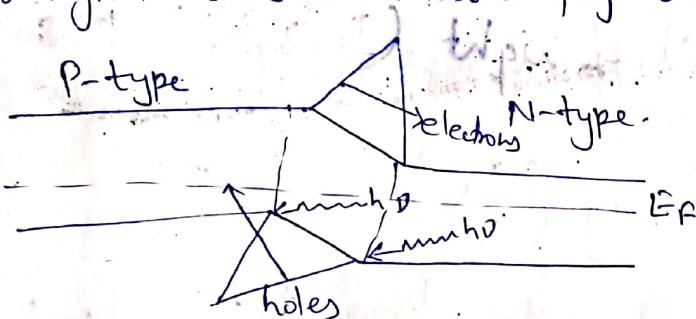


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#PHOTOVOLTAIC EFFECT - Process that generates voltage or electric current in a photovoltaic cell when it is exposed to sunlight. It is also defined as the effect due to which light energy is converted to electric energy in certain semiconductor materials.

In this process, e^- -hole pairs (mainly created in the depletion region and due to the built-in potential and electric field, e^- diffuse in the n-region & holes into the p-region as shown in the fig. below.



In general, net current flowing through the junction under the application of external voltage is

$$I_v = I_0 \left[\exp \left(\frac{eV}{k_b T} - 1 \right) \right] \quad \text{--- (1)}$$

where V may be +ve or -ve represents forward bias or reverse bias & I_0 = Dark current.

When light is allowed to fall on junction, photocurrent I_L is produced whose direction is opposite to that of I_v . The net current in the presence of light is ~~$I = I_v + I_L$~~ $I = I_L - I_v$ --- (2)

When no external voltage is applied, then the junction acts as a photo voltaic cell & $I=0$, so from eqn (2) we get

$$I_L + I_0 - I_0 \exp\left(\frac{eV_{ph}}{kT}\right) = 0 \quad (3)$$

where V_{ph} = photovoltage, so eqn (3) becomes,

$$\exp\left(\frac{eV_{ph}}{kT}\right) = \left(\frac{I_L + I_0}{I_0}\right) = \left(1 + \frac{I_L}{I_0}\right)$$

$$\text{or } \frac{eV_{ph}}{kT} = \log\left(1 + \frac{I_L}{I_0}\right) \text{ or } V_{ph} = \frac{kT}{e} \log\left(1 + \frac{I_L}{I_0}\right) \text{ --- (4)}$$

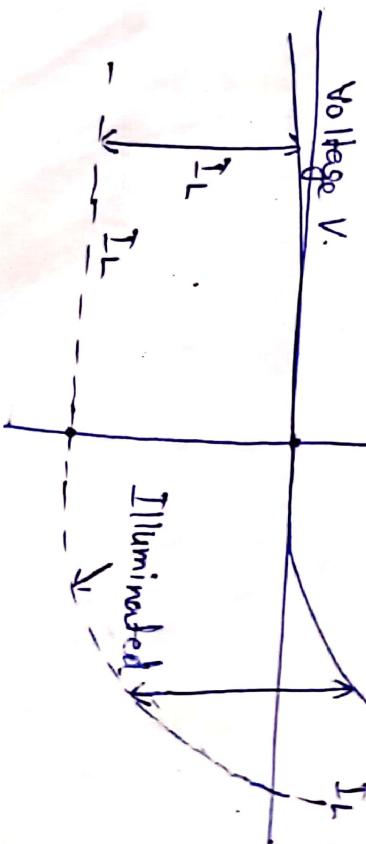
For high intensity of light ($I_L/I_0 \gg 1$) so we get

$$V_{ph} = \frac{kT}{e} \log\left(\frac{I_L}{I_0}\right) \quad (5)$$

The photovoltage varies logarithmically with the photo current and hence the intensity of E. M. radiation.

Current \uparrow

Dark

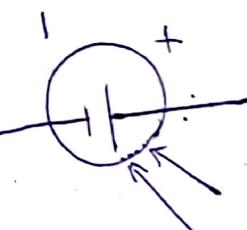


APPLICATION - SOLAR CELL

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A solar cell is a photovoltaic cell which converts the energy of light directly into electricity by the photovoltaic effect. This is a physical and chemical phenomena.



Symbol of photovoltaic cell.

Construction- It consists of a silicon PN junction diode with a glass window on top surface layer of p-material is made extremely thin, so that incident light photon's may easily reach the P-N junction.

When these photons collide with valence electrons, they impart sufficient energy to leave the

parent atoms. In this manner, free e⁻ and holes are generated on both the sides of the junction.

As a result, current is produced, which is directly proportional to the illumination ($\text{W/m}^2/\text{cm}^2$) and also depends on the size of the surface area being illuminated.

The surface exposed to sunlight is coated with anti-reflecting coating to avoid loss of incident light.

Metal contacts are made on n-type and p-type side (63) of sid semiconductor for electrical conduction.

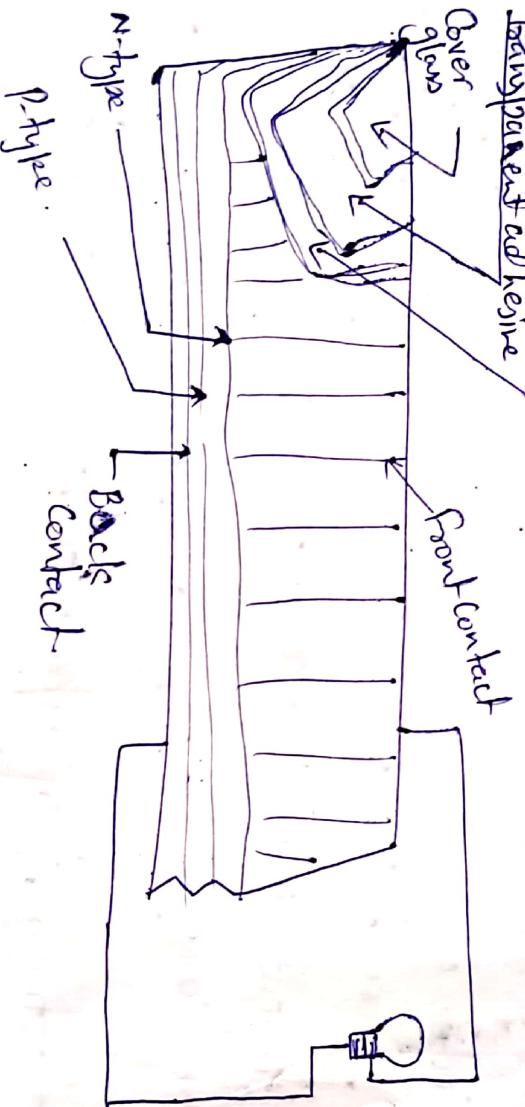
Working -

- (i) Photons are absorbed which generates e- & hole pairs in a semiconductor.

- (ii) e- & holes are separated to prevent recombination.

- (iii) When p-n junction is connected to the external circuit, the current flows.

Anti-reflecting coating.



As e- continues to diffuse more no. of negative charge on the emitter side and more no. of holes on the base side. is created.

The photovoltaic cell are connected electrically in series and in parallel to circuit to produce higher voltage and current. The PV cell produces 0.5-1V D.C.

Joint density of states in semiconductor:-

density of state for a semiconductor is defined the same way as for any material : (no. of energy states per unit volume in energy range E to $E + dE$) . For a semiconductor, however two or more bands can play role. Electrons in the conduction band and holes in the valence band . So , for a semiconductor, we used to calculate the joint density of states. i.e. the density of states in conduction band and the density of states in valence band .

Density of states is calculated for electron-hole pair having same wave vector (\vec{k}) which means only allowed transitions are considered. (not oblique.)

By using parabolic approximation,

$$E_2 = E_c + \frac{\hbar^2 k^2}{2m_c} \quad -(1)$$

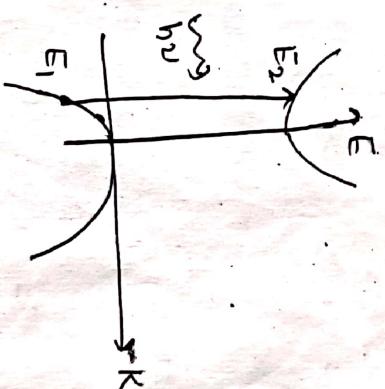
$$E_1 = E_v - \frac{\hbar^2 k^2}{2m_v} \quad -(2)$$

where, $E_c \rightarrow$ bottom edge of C.B. (Note \rightarrow free e^- energy

$$E_v \rightarrow m_c^*$$

so from eqn. (1) and (2)

$$\hbar v = E_g - E_1 = E_c + \frac{\hbar^2 k^2}{2m_c} - E_v + \frac{\hbar^2 k^2}{2m_v} \\ = (E_c - E_v) + \frac{\hbar^2 k^2}{2} \left(\frac{1}{m_c^*} + \frac{1}{m_v^*} \right) \quad -(3)$$



$\therefore E_c - E_v = E_g$
and $\frac{1}{m^*} + \frac{1}{m_v^*} = \frac{1}{m_r^*} \rightarrow$ reduced mass

So, eqn (3) =

$$\hbar\nu = E_g + \frac{\hbar^2 k^2}{2m_r^*}$$

$$\text{or } (\hbar\nu - E_g) = \frac{\hbar^2 k^2}{2m_r^*}$$

$$\text{or } k^2 = \frac{2m_r^*}{\hbar^2} (\hbar\nu - E_g)$$

Putting the value of k^2 in eqn (4), we have

$$E_g = E_c + \frac{\hbar^2}{2m_r^*} \cdot \frac{2m_r^*}{\hbar^2} (\hbar\nu - E_g) \quad (4)$$

$$E_g = E_c + \frac{m_r^*}{m_c^*} (\hbar\nu - E_g)$$

per unit volume

So, the no. of states in a range E_2 to $E_2 + dE_2$ per unit volume

can be written as (in conduction band)
 $g_c(E_2) dE_2 = g(\nu) d\nu \rightarrow$ no. of states, for photons of energy between $\hbar\nu$ & $\hbar(\nu + d\nu)$ to interact with

$$\text{So, } g(\nu) = \frac{g_c(E_2) dE_2}{d\nu} \quad (5)$$

$$\text{Hence } g_c(E_2) = \frac{1}{2\pi^2} \left(\frac{2m_c^*}{\hbar^2} \right)^{3/2} (E_2 - E_c)^{3/2} \quad (6)$$

$$\text{So, eqn (5) } \Rightarrow g(\nu) = \frac{1}{2\pi^2} \left(\frac{2m_c^*}{\hbar^2} \right)^{3/2} (E_2 - E_c)^{3/2} \frac{dE_2}{d\nu}$$

$$\text{from eqn (4)} \Rightarrow \frac{dE_2}{d\nu} = 0 + \frac{m_r^*}{m_c^*} \cdot \hbar$$

$$\text{Note } E_2 = E_c + \frac{m_r}{m_c} (\hbar\nu - E_g)$$

$$\left(E_2 - E_c \right)^{3/2} \left(\frac{m_r}{m_c} \right)^{3/2} g(\nu) = \frac{1}{2\pi^2} \left(\frac{2m_c^*}{\hbar^2} \right)^{3/2} (E_2 - E_c)^{3/2} \cdot \frac{\hbar}{2\pi^2} \frac{m_r^*}{m_c^*} \cdot \left(\frac{m_r}{m_c} \right)^{3/2} \cdot \left(\frac{2m_c^*}{\hbar^2} \right)^{3/2} \cdot \left(\frac{m_r^*}{m_c^*} \right)^{3/2} \cdot \left(\hbar\nu - E_g \right)^{3/2} \cdot \left(\frac{m_r^*}{m_c^*} \right)^{3/2}$$

$$\boxed{g(\nu) = \frac{1}{\pi\hbar^2} \cdot (2m_r^*)^{3/2} (\hbar\nu - E_g)^{3/2}}$$

DENSITY OF STATES FOR PHOTONS

⇒ Density of states for photons is the total number of allowed states per unit volume in the energy range E and $E+dE$

$$\rho(E) = \frac{dn(E)}{dE}$$



where $n(E)$ = no. of photons in phase-space having energy E

Note - phase space - A phase space is an imaginary space having 6 dimensions - 3 position & 3 momentum

3 position - x, y, z

3 momentum - p_x, p_y, p_z

It is described by position and momentum of each ~~particile~~ particle. It has minimum volume \hbar^3 .

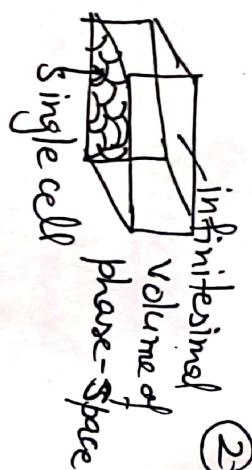
$dn(E) =$ no. of photons in infinitesimal phase space having energy in the range E & $E+dE$.

$\rho(E) =$ density of states for photons

According to phase-space concept.
if the no. of photons in infinitesimal volume is $dn(E) = d^3x d^3p / \hbar^3$

where $d^3x = dx dy dz$
 $d^3p = dp dq dy dz$

d^3p = infinitesimal volume of phase-space



$$\text{Therefore } d^3n(E) = \frac{\iiint d^3x d^3p}{h^3}$$

$d^3x d^3p$ = infinitesimal volume of phase-space

h^3 - volume of single cell

$$n(E) = \int d^3n(E) = \frac{V}{h^3} \int d^3p$$

$$\text{Now for } \int d^3p = \int_0^{2\pi} \int_0^\pi \int_0^{2\pi} p^2 dp \sin\theta d\theta \cdot d\phi$$

$$= \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \int_0^{2\pi} p^2 dp$$

$$= (2\pi)^x \int_0^\pi [-\cos\theta]^* x \int p^2 dp$$

$$= (2\pi)^x - (\cos\pi - \cos 0) \int p^2 dp$$

$$= 4\pi \int p^2 dp$$

$$\therefore n(E) = \frac{4\pi V}{h^3} \int p^2 dp$$

(2)

We have $E = pc$

$$p = E/c$$

$$dp = dE/c$$

$$\therefore n(E) = \frac{4\pi V}{h^3} \int \frac{E^2}{c^2} \frac{dE}{c}$$

$$= \frac{4\pi V}{h^3 c^3} \left(\frac{E^3}{3} \right)$$

According to pauli principle, for photon, in one state, two state polarization exists is

$$\therefore n(E) = 2 \times \frac{4\pi V}{h^3 c^3} \left(\frac{E^3}{3} \right)$$

$$= \frac{8\pi V E^3}{3 h^3 c^3}$$

Density of states for photons

$$f(E) = dn(E)/dE$$

$$f(E) = 3 \times \frac{8\pi V E^2}{3 h^3 c^3} = \frac{8\pi V E^2}{h^3 c^3}$$

Thus $f(nE) \propto E^3$ or $f(E) \propto E^2$

We also know $E = h\nu$

$$\therefore f(\nu) = \frac{8\pi(h\nu)^2 V}{h^3 c^3} = \frac{8\pi V \nu^2}{h c^3}$$

$$f(\nu) = n(\nu) = \frac{8\pi V (h\nu)^3}{h^3 c^3} = \frac{8\pi V \nu^3}{3 c^3}$$

Thus $\|n(\nu) \propto \nu^3 \& f(\nu) \propto \nu^2\| / 3 c^3$

(3)



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Computational approach to calculate optical excitations
Ex - Optical excitations in Boron Nitride (BN)

Optical process in solids - The method by which material interacts with material object is determined by the optical properties of the materials.

- Applications - (i) To design and build devices to manipulate light (mirrors, lenses, filters, polarizers etc) -
- (ii) With the help of optical properties of materials, one can obtain information about low energy excitations governing material physics.

Method

Energy for Excitation

(i) Thermal Excitation

(ii) Optical Excitation.

- (i) Thermal Excitation - (i) Electron-hole pairs are constantly generated by thermal as well as in the absence of any external energy source

- (ii) It does not require any scattering impulse.
- (iii) Caused by impurities, irregularities in structure lattice or by dopant.

- (iv) Strongly depend on E_{gap} .

- (v) Small E_g - increase in number of thermally excited charge -
- (vi) large E_g - low noise detector ex - Silicon ($E_g = 1.12 \text{ eV}$)
- (vii) Cooling is preferred to reduce noise.

Method

Optical Excitations -

- Energy of a single photon of visible light spectrum is comparable with band gap.
 - Photons of (λ) wavelengths 700nm - 400nm have energies 1.77 eV to 3.10 eV
 - Visible light is able to excite electrons to conduction band.
 - This is the principle of photovoltaic panels that generate electric current.
 - A quantum tho of optical excitation will drive solid at thermal equilibrium if $\text{two} \gg kT$ where T = temperature of solid.
- kT = mean energy'
- Optical interband transitions takes place
- After absorption, a number of electronic and vibrationally excited states populates & interact with each other.
 - Excitation relax towards equilibrium, through exchange of momentum and energy with rest of system.
 - Optically or electrically excited e- & holes with large excess energy $\Delta E \gg kT$ will interact themselves and with low lying excitations through very different processes.

Carrier lattice & Carrier-carrier interactions

- e- & holes interact mutually via Coulomb interaction & scatter off each other.
- Direct dissipation of excess energy into vibrational modes.
- Rate of such collisions (e-e, e-h, h-h) depends on carrier density & may involve either single-e- or collective excitations, like plasmons & phonons.
- Many of relevant reparation processes in the range of

Electronic Band Structure & Optical Excitations

Optical properties of semiconductors in the near infra-red visible and UV part of the spectrum are closely connected with their electronic band structure.

Gross feature of linear optical spectra

in the range $E_g < \text{thoc}$ 10eV can be obtained from (i) energy band structure $E(k)$ and the density of states derived from it (ii) the corresponding wave function ψ_{CR} of crystal e⁻ and (iii) fermi distribution function.

Many ion-electron system -

$$H_0 = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_{ij}|} + \sum_k \frac{p_k^2}{2M_k} + \frac{1}{2} \sum_{k \neq l} \frac{e^2}{|R_k - R_l|}$$

$$- \sum_{i, k} \frac{e^2}{|r_{ik}|}$$

Schroedinger equation for many body problem $\underbrace{\sum_{i,j} \frac{Z_i Z_j}{|r_{ij}|}}$ ion-ion interaction

$$H = -\sum_i \frac{\hbar^2}{2M_i} \nabla_i^2 - \sum_{i,m} \frac{\hbar^2}{2m_i} \nabla_i^2 + \frac{e^2}{2} \sum_{i,j \neq I} \frac{Z_i Z_j}{|R_i - R_j|}$$

(K.E. of ions) (K.E. of es)

$$+ \frac{e^2}{2} \sum_i \sum_{j,j \neq I} \frac{1}{|r_{ij}|} - e^2 \sum_I \sum_i \frac{Z_i}{|R_i - r_i|}$$

e-e interaction.

e-ion interaction.

Solving using Born-Oppenheimer approximation, we can calculate the true wave function and ground state energy. Transition from occupied valence to unoccupied conduction band states (upward transitions) and their time-reversed counter-parts (downward transitions)

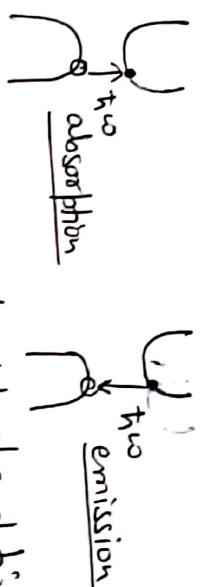


Fig A - Light absorption exciting the ground state of crystal.

Ex - Optical Excitation in Boron Nitride (BN)

It is demanding material of choice for emerging applications in optoelectronics electron emitters & detectors due to its high chemical stability, thermal conductivity, melting temperature, resistivity, band gap, optical absorption near the band edge ($\sim 7.5 \times 10^5$ cm $^{-1}$).

Optical properties of BN:-

- (a) Ultrathin Bandgap . (b) High optical emission & absorption (6.5 eV)

- c) Very large exciton energy - exciton binding energies is around 0.7 eV in BN Bulk crystals, & ~ 2.1 ev in BN - monolayers .

Excitations in N-e-system - In continuation of fig A.

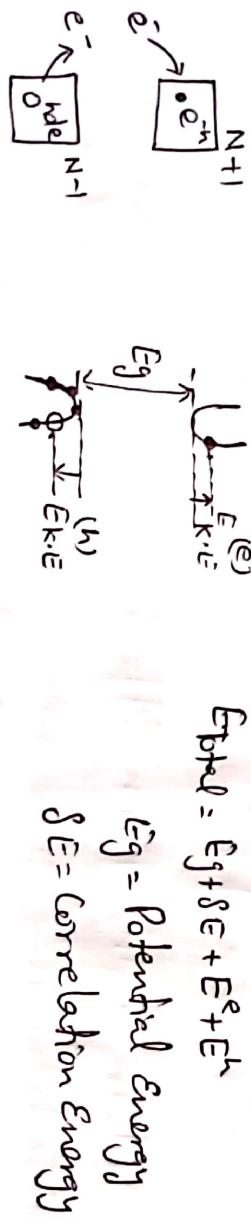


Fig B E-K diagram shows valence band &

conduction band with K-E-

During optical excitation Total Energy required $\Delta E = E_{\text{ex}} - E_0$
 $\Delta E = E_{\text{K.E}} + E_{\text{K.E}} + Eg - \delta E - E_0 \rightarrow$ Ground State Energy -
 K.E of e-hole

Coulomb Correlation

⑤

In general, three different types of correlated e-h pair motion may be expected when "excitons" are excited in a semiconductor.

- (i) Excited e- does not leave the atomic site of its origin & stay bound to it (self trapped exciton).
- (ii) Both e- & holes are mobile after excitation but remain in a bound ~~site~~ state relative to each other.
- (iii) e- & hole are unbound.

Ans.



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Finite Element Method — A numerical technique to find approximate solutions of partial definite equations. It helps in producing stiffness and strength visualizations. It also helps to minimize material weight & cost and its cost of structures. It allows entire design to be constructed, refined & optimized before the design is manufactured. This tool has noticeably improved the engineering design standard and methodology of the design process in many industrial applications.

Numerical Methods — Commonly used numerical methods to solve solid & fluid mechanics problem are

- Finite Difference Method
- Finite volume method
- Finite element method
- Boundary Element Method
- Meshless method

Finite element method is in general a numerical method for solving partial differential equations in two or three dimensions. For solution, a large system is divided into smaller, simple parts called 'finite elements'.

Why? It provides, safe simulation of potentially dangerous or destructive local conditions & failure modes, allowing engineers to discover a system's physical response to any location.

Finite Element Method - Photon Density of States (In-plane)

To find the photon density of states, the dispersion relation [relates the wavelength and wavenumber of a wave to its frequency]. With the dispersion relation, the phase velocity & group velocity of waves in a medium, as a function of frequency can be calculated. not only at boundaries but also in the interior of irreducible Brillouin zone are needed.

Dispersion relation for triangular lattice, the dimensionless frequency is calculated as a function of Bloch's vector as in the interior parts of irreducible Brillouin zone. Then the dispersion relations can be plotted as 3D diagrams which will be a surface for each band. To get the in-plane PDOS calculation, by definition we have $dN(\omega) = D(\omega) d\omega$. Equationally, the expression for PDOS is

$$D(\omega) = \frac{S}{4\pi^2} \int_{\omega_k} \sqrt{1 + \left(\frac{\partial \omega}{\partial k_x}\right)^2 + \left(\frac{\partial \omega}{\partial k_y}\right)^2} dk_x dk_y.$$

Steps involved in FEM

(3)

1. Divide the interval of integration - Numerical result is an approximation to exact soln.
2. Each sub-interval, select a proper functions to emulate the true function - accuracy of numerical result depends on the number of sub-interval & approximate function.

On a software systems FEA requires following information -

- 1- Nodal points spatial locations
- 2- Elements connecting nodal points-
- 3- Mat properties & boundary restraints-
- 4- Loading function details
- 5- Analysis Options-

Applications -

- Mechanical Engg. design
- Structural Analysis
- Solid Mechanics
- Modal analysis
- Fatigue & Fracture Mechanics
- Computer Aided
- Thermal & Electrical analysis
- Computer Aided
- Drafting (CAD) and Engineering Simulations Services

$$x \longrightarrow x \longrightarrow x$$

Numerical computation of optical loss -

OPTICAL LOSS → It can be introduced by blocking the light ray radiating out from the input fiber routed to the output fiber.

In case of optical fiber, there is an exponential loss of launched power in the fiber. If P_0 is the power launched at the input point of the fiber of length L , the transmitted power P_T is given by

$$P_T = P_0 e^{-\alpha L}$$

where α is the attenuation constant which is referred as fiber loss.

Optical loss chiefly affect the power from a solar cell by lowering the short-circuit current. Optical loss consist of light which could have generated an e-hole pair, but does not, because the light is reflected from the front surface, or because it is not absorbed in the solar cell.

Types of optical loss in a Solar Cell - (Thin film Solar Cell)

In thin-film Solar cell, optical losses are due to
 (i) Non-absorption (ii) Thermalization (iii) Reflection
 (iv) Transmission & area loss.

(i) Non-absorption — In this, the photons with energy less than the band gap of energy of absorbing material are transmitted as a result such photon energy is lost due to non-absorption.

(iv) Thermalization - When $E_{ph} > E_g$, leads to thermalization.

It occurs for photons which have energy higher than band gap. Excess amount of energy is dissipated as heat, as a result it increases the temperature of the solar cell. ($E_{ph} - E_{gap}$)

(v) Reflection loss - It occurs due to blocking of light by top contact, reflection from top surface & reflection from back contact without proper absorption. Also called as reflection loss.

(vi) Transmission & Area loss - It is due to finite thickness of cell and the effect is enhanced in materials having low absorption coefficient.

* Formula for Reflection loss -

$$\text{Return loss (dB)} = -10 \cdot \log \frac{\text{Forward power}}{\text{Reflected power}}$$

$$\text{Return loss (dB)} = -20 \lg |r|$$

$$\text{Reflection Coefficient } r = 10 - \frac{\text{Return loss}}{20}$$

Numericals on Unit 2 & 3

Q1. Consider that in an n-type GaAs semiconductor at 300K temperature, the e⁻ concentration varies linearly from 1×10^{18} to 7×10^{17} cm⁻³ over a distance of 0.10cm. So, calculate the diffusion current density if e⁻ diffusion coefficient is $D_n = 225$ cm²/s.

Soln1. Diffusion Current density is

$$J_{\text{diff}} = e D_n \frac{dn}{dx} \approx e D_n \frac{\Delta n}{\Delta x}$$

So, on per value

$$J_{\text{diff}} = 1.6 \times 10^{-19} \times 225 \times \frac{(1 \times 10^{18} - 7 \times 10^{17})}{0.10}$$

$$= 108 \text{ A/cm}^2 \quad \underline{\text{Ans}}$$

Q2. Consider a p-type Si sample for which the hole diffusion coefficient is 9 cm²/sec. If the hole concentration varies from 10^6 cm⁻³ to 10^{13} cm⁻³ over a length of 1 mm, then find out the diffusion current density.

Soln2- Diffusion current density is given by

$$J_{\text{diff}} = \rho D_p \frac{dp}{dx} \approx \rho D_p \frac{\Delta p}{\Delta x}$$

$$= 1.6 \times 10^{-19} \times 9 \times \frac{(10^{16} - 10^3)}{1 \times 10^{-6} \times 100}$$

$$= 143.86 \text{ A/cm}^2 \quad \underline{\text{Ans}}$$

Q3. Find the position of fermi level E_F at room temperature (2) nature ($= 27^\circ C$) for Germanium crystal having 5×10^{22} atoms/m³

Ans3: Given $T = 27^\circ C = 300K$ and $n_e = 5 \times 10^{22}$ atoms/m³

$$n_e = 2 \left(\frac{2\pi m_e^* kT}{h^2} \right)^{3/2} e^{(E_F - E_c)/kT}$$

$$= e^{(E_F - E_c)/kT} = \frac{n_e}{2 \left(\frac{2\pi m_e^* kT}{h^2} \right)^{3/2}}$$

$$= e^{(E_F - E_c)/kT} = \frac{5 \times 10^{22}}{\left[\frac{2 \times 3.14 \times 9.1 \times 10^{-31} \times 1.38 \times 10^{-23} \times 300}{(6.62 \times 10^{-34})^2} \right]^{3/2}}$$

$$= e^{(E_F - E_c)/kT} = \frac{5 \times 10^{22}}{25.0115 \times 10^{24}}$$

$$e^{-(E_c - E_F)/kT} = 0.1991 \times 10^{-2}$$

$$e^{-(E_c - E_F)/kT} = 502.296 \text{ or } E_c - E_F = \log 502.296$$

$$\frac{E_c - E_F}{kT} = 6.2192 \text{ or } E_c - E_F = 0.161 eV$$

③

Q4 - For an intrinsic Semiconductor having band gap $E_g = 0.7\text{ eV}$ calculate the density of holes and electrons at room temperature ($= 27^\circ\text{C}$). Given $\hbar = 6.62 \times 10^{-34}\text{ J s}$, $m = 9.1 \times 10^{-31}\text{ kg}$

$$\pi = 3.14 \quad k = 1.38 \times 10^{-23}$$

Solution - Given $E_g = 0.7\text{ eV}$

In intrinsic semiconductor the concentration of electrons and holes are same. So

$$n_e = n_h = 2 \left[\frac{2\pi k T m}{h^2} \right]^{3/2} e^{(E_F - E_C)/kT}$$

The Fermi level lies exactly in between the middle of conduction and valence band.

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

$$E_F - E_C = \frac{E_C + E_V - E_C}{2} = \frac{(E_C - E_V)}{2} = -\frac{E_g}{2}$$

$$\therefore n_e = n_h = 2 \left[\frac{2\pi k T m}{h^2} \right] e^{-E_g/2kT}$$

$$= 2 \times \left[\frac{2 \times 3.14 \times 1.38 \times 10^{-23} \times 300 \times 9.1 \times 10^{-31}}{6.62 \times 10^{-34}} \right] e^{-\left[\frac{0.7}{2 \times 0.026} \right]}$$

$$= 3.6 \times 10^{19} / \text{m}^3.$$



Q5 - A single solar cell (10cm x 10cm) produces a voltage of 0.5V and a current upto 0.25A. If the solar insulation is 800 W/m^2 , find the efficiency of solar cell?

Soln 5 - Surface Insulation (S.I.) = 800 W/m^2 , V = 0.5V, I = 2.5A, $\eta = ?$

$$\eta = \frac{P_{\text{out}}}{P_{\text{in}}} \times 100$$

where $P_{\text{out}} = \text{Voltage (V)} \times \text{current (I)}$

$$P_{\text{in}} = S \cdot I \times \text{area}$$

$$\eta = \frac{V \cdot I}{S \cdot I \times \text{area}} = \eta = \frac{0.5 \times 2.5}{800 \times 10^{-2}}$$

$$\eta = 0.1562 = 15.62\%$$

Q6 - Solar insulation on a rectangular module (1.5m x 2.0m) of photovoltaic cell is 550 W/m^2 . If the efficiency of cell is 12%. What is the power output of the module?

$$\underline{\text{Soln 6}} - \eta = \frac{P_{\text{out}} \times 100}{P_{\text{in}}} =$$

$$\eta = \frac{P_{\text{out}}}{\text{Area} \times S \cdot I} =$$

$$0.12 = \frac{P_{\text{out}}}{550 \times 3} = 0.12 \times 550 \times 3$$



Q7. Calculate the drift velocity of e^- in an aluminium wire of diameter 0.9 mm carrying current of 6 A. Assume that $4.5 \times 10^{28} \text{ el./m}^3$ are available for conduction.

$$\text{Soln} - I = 6 \text{ A}, n = 4.5 \times 10^{28} \text{ el./m}^3 \text{ & radius } (r) = \frac{d}{2} = \frac{0.9 \times 10^{-3}}{2}$$

$$= 4.5 \times 10^{-4} \text{ m}$$

$$\begin{aligned} J &= \frac{I}{A} \\ (\text{Current Density}) &= \frac{6.0}{\pi \times (4.5 \times 10^{-4})^2} \\ &= 9.44 \times 10^6 \text{ A/m}^2 \\ &= \frac{9.44 \times 10^6}{3.14 \times (4.5 \times 10^{-4})^2} \\ &\text{ & drift velocity } v_d = \frac{J}{n e} = \frac{9.44 \times 10^6}{4.5 \times 10^{28} \times 1.6 \times 10^{-19}} \\ &= 1.311 \times 10^{-3} \text{ m/sec.} \end{aligned}$$