# Unit - 3

1. Concept of optical transitions in bulk s.c :-

Among energy states, the state with the lowest energy is most stable. Therefore the electrons in s.c. tend to stay in low energy states. If they are excited by thermal energy, light or electron beams the electrons absorb these energies and transit to Higher energy states. These transitions of the electrons from low energy state to high energy state are called excitations. High energy states however are unstable. As a result, to take stable states the electrons in high energy states transit to low energy states in certain life times.

These transitions of the excited electrons from high energy states to low energy states are reffered as relaxations.

| E_c —————— | E_c ——↑——— | E_c ——↓——— | —————— E_c |
| Stable state | E_V Excitation | E_V Relaxation | stable state |
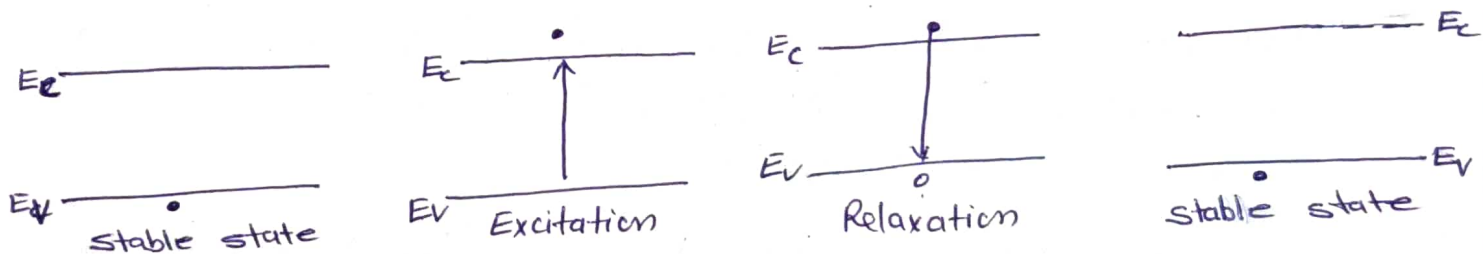
2. Optical absorption process:-

If a wide range of electromagnetic energy is consumed by the valance electron, the excited electrons go to various energy levels of the conduction band. Besides this, there are several mechanism of absorbtion by which electrons (and holes) absorb optical energy.

But for bulk s.c we generally discuss band to band transitions.

In band to band transsition, an electron in the V.B absorbs a photon with enough energy to be excited to the conduction band leaving a hole behind.

These band to band transitions, can further categorised as direct and indirect band gap transitions. In direct band gap materials, the energy transitions is more direct means no change occurs in momentum. Whereas in indirect band gap materials, large change in momentum occurs.

(a) <mark>Direct band gap absorption transition</mark> :-

Let us consider the transition of the electrons from the top of V.B to the bottom of C.B. A sc, in which <mark>top of V.B and bottom of C.B are placed at the common wave vector K</mark> is direct transition s.c.
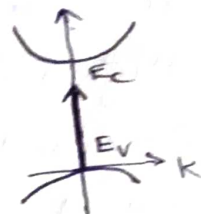
In transition of electrons, the energy and momentum are conserved. Therefore phonon do not take part in direct transition. because the wave vector K of the phonons is much longer than that of photon. Hence in the direct transition the transitions Probabilities are determined by only the electrons transition Probabilities.

The absorption coefficient for direct band gap absorption can be written as.
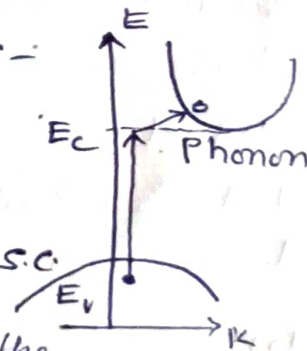
$$\alpha(\hbar\omega) = A(\hbar\omega - E_g)$$

↓ Absorption Coefficient

↓ Magnetic Vector Part.

(b) <mark>Indirect band gap absorption transition</mark> :-

A sc, in which the bottom of Conduction band and the top of valance band have different K-values is the indirect transition s.c.

The phonon transition accompany to satisfy the momentum conservation law. so

Transition Probability = electron transition Probability × Phonon transition probabilities.

$$\alpha(\hbar\omega) = A^2(\hbar\omega - E_{ph})^2 \to \text{Energy of phonon.}$$ Phonon transition

where $B_{12} \rightarrow$ is a probability constant called ei Einstein's coeffici for absorption process. and depends upon the properties of state or energy level E_1 and E_2.

Emission process :- when the atom is in the excited state it can make a transition to a lower energy state through the emission of EM radiation. The emission can occur in two different way.

1. Spontaneous emission

2. Stimulated emission

Spontaneous emission :- when an atom in excited state emits radiation

spontaneously, in absence of any incident radiation. The process is known as spontaneous emission of radiation.

The rate of spontaneous emission or probability of emission is proportional to the no. of atom in excited state i.e N_2

$(P_{21})_{spon} \propto N_2$

or $\boxed{(P_{21}) = A_{21} N_2}$ ← (Spontaneous emission rate)

$A^* \rightarrow A + \hbar \nu$
(Spontaneous emission)

where $A_{21} \rightarrow$ Einstein's coefficient of spontaneous emission of radiation.

Stimulated Emission :- when an atom is in the excited state, then an incident photon

of current energy ($\hbar \nu = E_2 - E_1$) may cause the atom to jump to lower energy state, emitting an additional photon of same frequency are present.

This process is called stimulated emission of radiation

The rate of stimulated emission Probability of emission depends both intensity of external radiation and on no. of atom in upper level N_2.

$A^* + \hbar \nu \xrightarrow{\text{Sti emission}} A + 2\hbar \nu$
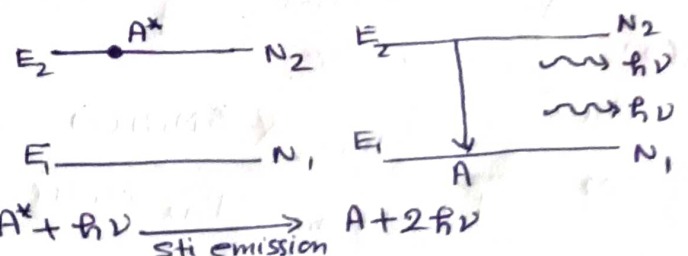
Concept of Recombination Process:-

In semi conductors the transition of electrons from high energy states to low energy states are designated recombination of electrons and holes.

There are radiative and non radiative recombination.

The radiative recombinations emit photons, and the energy of photons correspond to the difference b/w initial and final energy states.
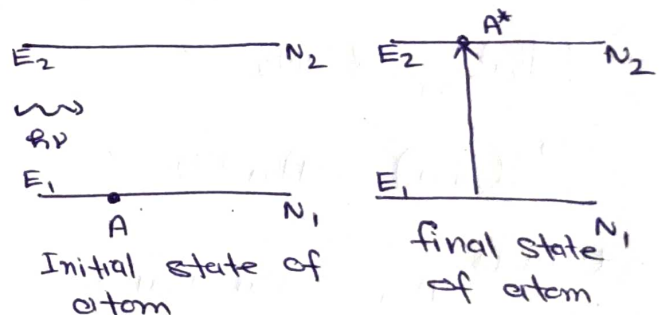
In the non radiative recombination, the photon are emitted to the crystal lattice or the electrons are trapped in the defects, and the transition energy is transformed into form other than light.

Stimulated Absorption:-

An atom has a no. of quantized energy states.

Initially an atom is in the ground state. i.e all of its electrons possess the lowest energy state.

When energy is given in the form of EM radiation, the atom goes to the excited state (higher energy state) by absorbing a quanta or photon.

E_2 ———— N_2 E_2 $\uparrow$ A^* ———— N_2

$\sim\sim$
$R\nu$

E_1 ————•———— N_1 E_1 ———————— N_1

A
Initial state of atom   final state of atom

This process is called stimulated absorption or induced absorption. if E_1 and E_2 are initial and final energy state then

$$E_2 - E_1 = h\nu$$

$$\nu = \frac{E_2 - E_1}{h}$$

$$h\nu + A \xrightarrow[\text{Absorption}]{\text{Stimu}} A^* \text{ (excited) atom}$$
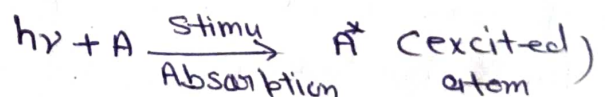
The probability of absorption depends on energy density $u(\nu)$ of radiation

Thus $(P_{12})_{Sti. Abs} \propto N_1 u(\nu)$

or $\boxed{(P_{12})_{Sti. Abs} = B_{12} \cdot N_1 u(\nu)}$ ← (stimulated absorption rate)

$$(P_{21})_{sti. emi} \propto N_2 \, u(\nu)$$

$$\boxed{(P_{21})_{sti. emi} = B_{21} \, N_2 \, u(\nu)} \leftarrow \text{stimulated emission rate.}$$

where $B_{21} \rightarrow$ Einstein's coefficient of stimulated emission of radiation.

Hence total probability of emission

$$(P_{21})_{emission} = (P_{21})_{spon} + (P_{21})_{sti}$$

$$\boxed{(P_{21})_{emission} = [A_{21} + B_{21} u(\nu)] N_2}$$

==Optical transition in thermal equilibrium :-==

==(Relation b/w Einstein's coefficient) :-==

Consider an assembly of atoms in thermal equilibrium at temperature T with radiation of frequency ν and energy density $u(\nu)$. Let N_1 and N_2 be the no. of atoms in energy state 1 and 2 respectively at any instant.

Probability of absorption is given by

$$P_{12} = B_{12} \, N_1 \, u(\nu) \longrightarrow (1)$$

and total probability of emission is given by

$$P_{21} = [A_{21} + B_{21} \, u(\nu)] N_2 \longrightarrow (2)$$

At equilibrium Absorption and emission rate must be equal.

$$B_{12} \, N_1 \, u(\nu) = A_{21} N_2 + B_{21} N_2 \, u(\nu)$$

$$u(\nu) [N_1 B_{12} - N_2 B_{21}] = A_{21} N_2$$

$$u(\nu) = \frac{A_{21} N_2}{N_2 B_{21} \left[\left(\frac{N_1}{N_2}\right)\left(\frac{B_{12}}{B_{21}}\right) - 1\right]} \longrightarrow (3)$$

$$u(\nu) = \frac{A_{21}}{B_{21} \left[\left(\frac{N_1}{N_2}\right)\left(\frac{B_{12}}{B_{21}}\right) - 1\right]} \longrightarrow (3)$$

at equilibrium $\boxed{B_{12} = B_{21}}$

$$u(\nu) = \frac{A_{21}}{B_{21}\left(\frac{N_1}{N_2} - 1\right)} \longrightarrow (4)$$

A/c to Boltzmann distribution law, the no. of atom N_1 and N_2 in energy states E_1 and E_2 in thermal equilibrium at temp T. are given by

$$N_1 = N_0 \, e^{-E_1/kT} \quad \text{and} \quad N_2 = N_0 e^{-E_2/kT}$$

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

$$= e^{h\nu/kT} \qquad \qquad \therefore E_2 - E_1 = h\nu$$

then

$$u(\nu) = \frac{A_{21}}{B_{21}\left(e^{h\nu/kT} - 1\right)} \longrightarrow (5)$$

Comparing equation (4) with planck's radiation formula

$$u(\nu) = \frac{8\pi h \nu^3}{c^3} \cdot \frac{1}{\left(e^{h\nu/kT} - 1\right)} \longrightarrow (6)$$

from (5) and (6)

$$\boxed{\frac{A_{21}}{B_{21}} = \frac{8\pi h \nu^3}{c^3}} \longrightarrow (8)$$

$$\boxed{B_{21} = B_{12}} \quad \text{and} \quad \boxed{\frac{A_{21}}{B_{21}} = \frac{8\pi h \nu^3}{c^3}} \quad \text{are called einstein's relations.}$$

Joint density of states in Semi conductor:- Density of states for a semiconductor is defined the same way as for any material : (no. of energy state per unit volume in energy range E to $E+dE$). for a semiconductor, however two or more bands can play role, electrons in C.B and holes in V.B. So, for a semiconductor, we used to calculate the joint density of states. i·e the density of states in C.B and V.B:—

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

By using parabolic approximation

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

$$E_1 = E_v - \frac{\hbar^2 k^2}{2m_v^*} \longrightarrow (2)$$
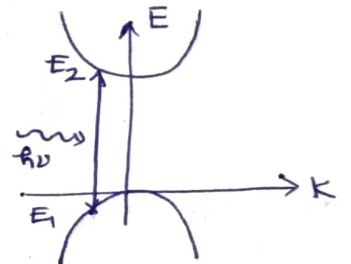
$$\therefore \left(E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \right) \quad \hbar\nu = E_2 - E_1$$

where $E_c \to$ bottom edge of C.B

$E_v \to$ Upper edge of V.B

m_c^* and $m_v^* \to$ effective mass of e^- and holes in C.B and V.B resp.

So from equation (1) and (2)

$$\hbar\nu = E_2 - E_1 = E_c + \frac{\hbar^2 k^2}{2m_c^*} - E_v + \frac{\hbar^2 k^2}{2m_v^*}$$

$$\hbar\nu = (E_c - E_v) + \frac{\hbar^2 k^2}{2}\left(\frac{1}{m_c^*} + \frac{1}{m_v^*}\right) \longrightarrow (3)$$

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

Let·

$$\therefore \frac{1}{m_c^*} + \frac{1}{m_v^*} = \frac{1}{m_\sigma^*}$$

(Reduced mass)

$$\hbar\nu - E_g = \frac{\hbar^2 k^2}{2m_\sigma^*}$$

Or $$k^2 = \frac{2m_\sigma^*}{\hbar^2}(\hbar\nu - E_g)$$ Put this value in eqn (1) we get

$$E_2 = E_c + \frac{\hbar^2}{2m_c^*} \cdot \frac{2m_\sigma^*}{\hbar^2}(\hbar\nu - E_g)$$

$$E_2 \neq E_c + \frac{m_\sigma^*}{m_c^*}(\hbar\nu - E_g) \longrightarrow (4)$$

So the no. of state per unit volume in a range E_2 to $E_2 + dE_2$ can be written as (in conduction band)

$$g_c(E_2) dE_2 = g(\nu) d\nu \rightarrow \text{no. of states per unit volume for photons of energy b/w } \hbar\nu \text{ & } \hbar(\nu+d\nu) \text{ to intract with.}$$

So. $g(\nu) = \dfrac{g_c(E_2) dE_2}{d\nu}$ ⟶ (5)

Here $g_c(E_2) = \dfrac{1}{2\pi^2}\left(\dfrac{2m_c^*}{\hbar^2}\right)^{3/2}(E_2 - E_c)^{1/2} \cdot \dfrac{dE_2}{d\nu}$

from eqⁿ (4) ⟹ $\dfrac{dE_2}{d\nu} = 0 + \dfrac{m_\sigma^*}{m_c^*} \cdot \hbar$

So. $g(\nu) = \dfrac{1}{2\pi^2}\left(\dfrac{2m_c^*}{\hbar^2}\right)^{3/2}(E_2 - E_c)^{1/2} \cdot \hbar \dfrac{m_\sigma^*}{m_c^*}$

$= \dfrac{1}{\pi\hbar^2}(2m_c^*)^{3/2}\left(\dfrac{m_\sigma^*}{m_c^*}\right)^{1/2}(\hbar\nu - E_g)^{1/2} \cdot \left(\dfrac{m_\sigma^*}{m_c^*}\right)$

$$\boxed{g(\nu) = \dfrac{1}{\pi\hbar^2}(2m_\sigma^*)^{3/2}(\hbar\nu - E_g)^{1/2}}$$

optical gain in a semi conductor :-

The optical joint density of states takes into account the no. of states available in both C.B and V.B with which a photon of energy $\hbar\nu$ can intract and given by.

$$P(\nu) = \dfrac{(2m_\sigma)^{3/2}}{\pi\hbar^2}(\hbar\nu - E_g)^{1/2} \quad ; \quad \hbar\nu \geqslant E_g \longrightarrow (1)$$

Note that only photons with energy $\hbar\nu \geqslant E_g$ can participate in the emission and absorption process.

if $\hbar\nu = E_2 - E_1$ is the energy of an incident photon then for absorption of the photon, an electron should be present in the state with energy E_1 in the V.B and there should be an unoccupied allowed state at energy E_2 in C.B. Thus the probability of absorption is given by (in quasi-equilibrium),
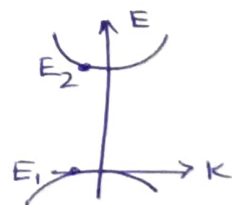
$$P_a(\nu) = \underset{\downarrow}{f_v(E_1)}[1 - f_c(E_2)] \longrightarrow \underset{②}{\text{Probability that a state with energy } E \text{ remains unoccupied.}}$$

Probability of occupation of state E.

Similarly, for emission of photon, it requires that an electron exists at energy level E_2 in the C.B and there exists a hole at energy level E_1 in V.B.

Therefore, the <u>probability of emission</u>.

$$P_e(\nu) = f_c(E_2)[1-f_v(E_1)] \longrightarrow (3)$$

for net emission, we must have $P_e(\nu) > P_a(\nu)$

or

$$f_c(E_2)[1-f_v(E_1)] > f_v(E_1)[1-f_c(E_2)] \longrightarrow (4)$$

$$P_e(\nu) = \left[\frac{1}{e^{(E_2-E_{F_c})/kT}+1}\right]\left[\frac{e^{(E_1-E_{f_v})/kT}}{e^{(E_1-E_{f_v})/kT}+1}\right] \longrightarrow (5)$$

and

$$P_a(\nu)\left[\frac{1}{1+e^{(E_1-E_{Fv})/kT}}\right]\left[\frac{e^{(E_2-E_{Fc})/kT}}{1+e^{(E_2-E_{Fc})/kT}}\right] \longrightarrow (6)$$

from eq^n (5) and (6) $\Rightarrow$

$$e^{(E_1-E_{fv})/kT} > e^{(E_2-E_{Fc})/kT}$$

or. $\quad E_1 - E_{F_v} > E_2 - E_{FC}$

$$E_{FC} - E_{FV} > E_2 - E_1 = \hbar\nu$$

$$\boxed{E_{fc} - E_{fv} > E_g} \longrightarrow (7)$$

when the separation b/w quasi-fermi levels in a s.c exceeds the band gap, then for all frequencies ν that satisfy eq^n (7), it is possible to have <u>light amplification</u> or <u>overall optical gain</u>.

The gain coefficient for amplification of radiation of frequency ν by stimulated emission in a s.c is given by

$$\gamma(\nu) = \frac{(c/n)^2}{8\pi \tau_n} \frac{\rho(\nu)}{\nu^2} \cdot \Delta P \longrightarrow (8)$$

Where
$\tau_n \rightarrow$ recombination time
$\rho(\nu) \rightarrow$ Joint density of state
$\Delta P = P_e(\nu) - P_a(\nu)$

for amplification, $\gamma(\nu) > 0$ which requires $\Delta P > 0$ i.e the probability of emission has to be greater than the probability of absorption.

Optical loss or absorption coefficient in thermal equillibrium :-

A semiconductor in thermal equilibrium has only a single fermi level i.e. $E_F = E_{Fc} - E_{FV}$

and the carrier distribution is given by the fermi function and therefore both $f(E_1)$ and $[1 - f(E_2)]$ are much larger than $f(E_2)$ and $[1 - f(E_1)]$. Thus

$$P_e(\nu) < P_a(\nu)$$

also
$$\Delta P = P_e(\nu) - P_a(\nu) = -ve.$$

Therefore, the gain coefficient $\gamma(\nu)$ in eq^n (8) is always negative. (Since $E_2 > E_1$).

Thus, a semiconductor in thermal equilibrium, whether it is intrinsic or doped, always attenuates light and we have the overall optical loss in semiconductor.