Semiconductor Physics and Computational Methods (21PYB102J)

Course Instructor: **Dr. Venkata Ravindra A**
Assistant Professor
Department of Physics and Nanotechnology
SRM Institute of Science and Technology
Email: **venkatar1@srmist.edu.in**
Phone: **8019448666**
Office: **UB-709/A**

DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

21PYB102J –Semiconductor Physics and Computational Methods

Module III

- For the optical properties of semiconductors, the photons should interact with charge carriers.
- In the process of interaction three process occurs
  - **Absorption**
  - **Recombination**
  - **Emission**

i.e the photons are absorbed and emitted , these processes are important in photonic devices using semiconductors
There are several type of transition possibilities to occur

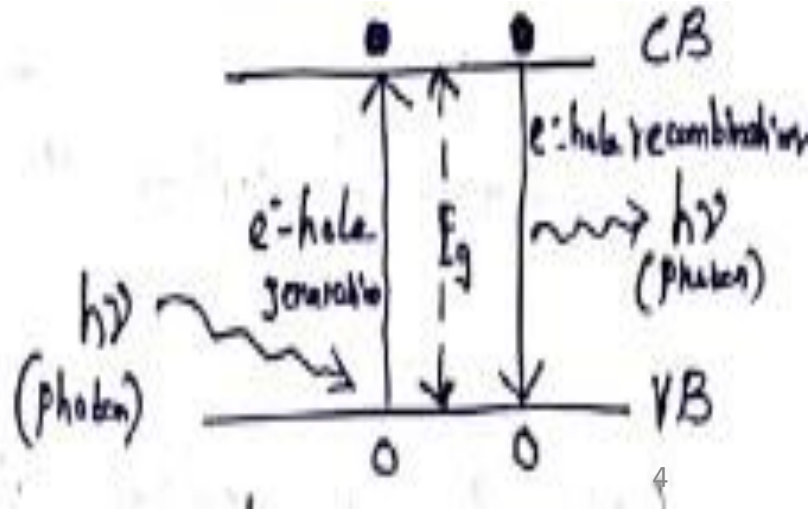
1. **Band to band transition (Inter band transition)**
2. **Impurity level to band transition**
3. **Free carrier transition (Intra band transition)**

In semiconductors, electrons can make transitions between two energy states and create or destroy photons in the process.

1. Band to band transition (Inter band transition)

An absorbed photon can result in an electron in the valence band making an upward transition to conduction band. This results electron-hole pair generation, followed by this electron-hole recombination takes place by the emission of Photon

Eg: Band to Band transition in GaAs can results absorption and emission of photons with wavelength of 0.087 μm or (E_g = 1.42 eV)



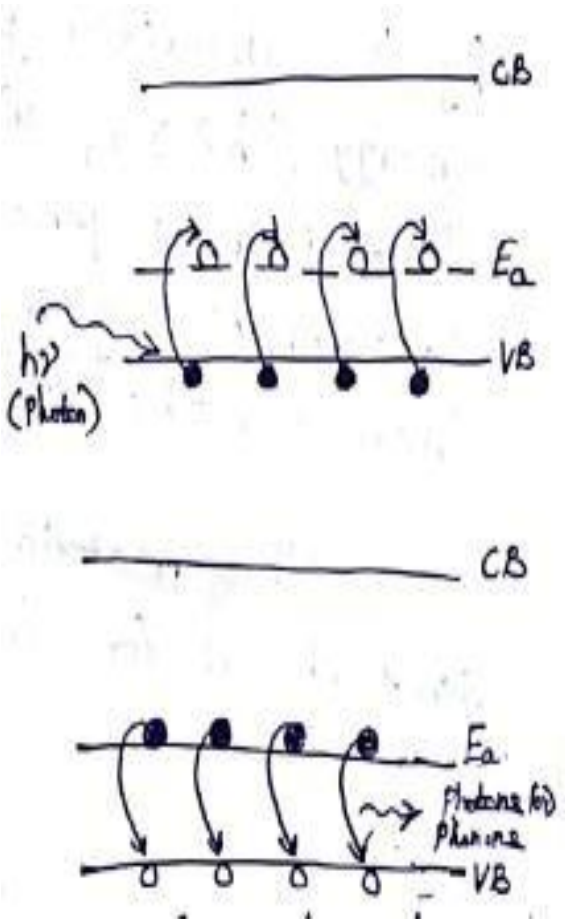
2. Impurity level to band transition:

An absorbed photon results in a charge carriers transition between a donor (or) acceptor level to a band in semiconductor, mostly observed in doped semiconductors.

For example if a p-type material is considered, the low energy photon absorbed by p-type semiconductor material leads transition of electron from valence band to acceptor level where its trapped by acceptor atom. Thus hole is created in Valence band and acceptor atom is ionized.

Similarly a hole may be trapped by an ionized acceptor atom. The result may be the electron decay from its acceptor level to recombine with hole. The energy may be released radiatively (photons) or non-radiatively (phonons)

Eg: In Hg doped Ge the wavelength of absorption and emission between valence and conduction band is 14 μm

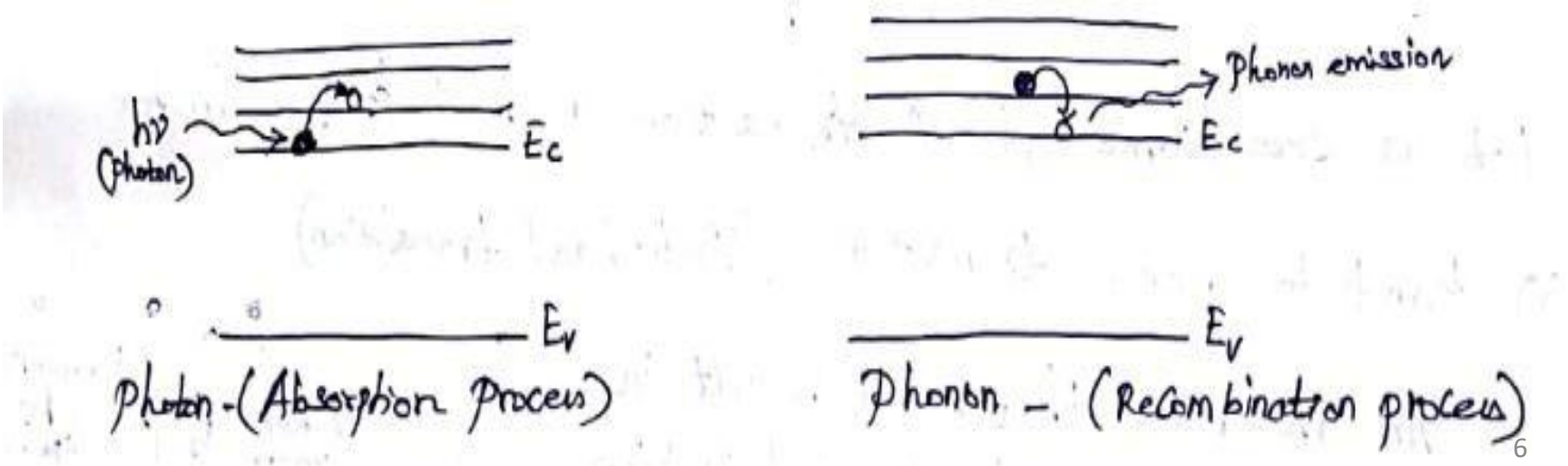


3. Free carrier transition (Intra band transition):

An absorbed photon can impart its energy to an electron in a given band, causing it to move to higher level in that band.

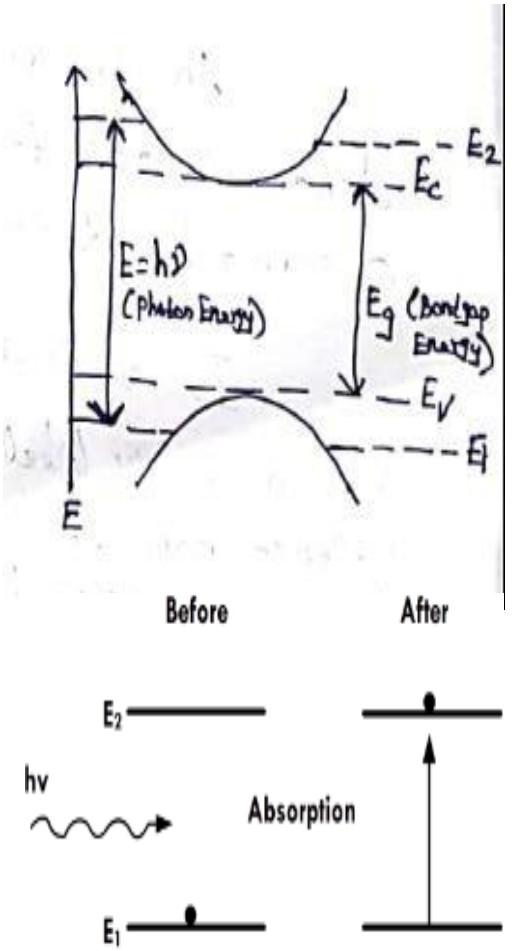
If a lower level conduction band is considered, by absorbing photon energy the electron moves to next higher energy level in the same conduction band.

Similarly due to thermalization, electron relaxes down to the bottom of the conduction band while releasing its energy in the form of phonons.



Optical absorption process :

Absorption is the process in which the photons absorbed by the semiconductor materials causes transition of electron from valence band to conduction band.



Consider direct band to band absorption:

The condition for absorption to happen, the incident photon energy must be equal Or grater than the bandgap i.e $h\nu \geq E_g$, corresponding wavelength $\lambda = hc/E_g$.

The electron hole pairs are generated due to absorption of photon having energy grater Or equal to bandgap.

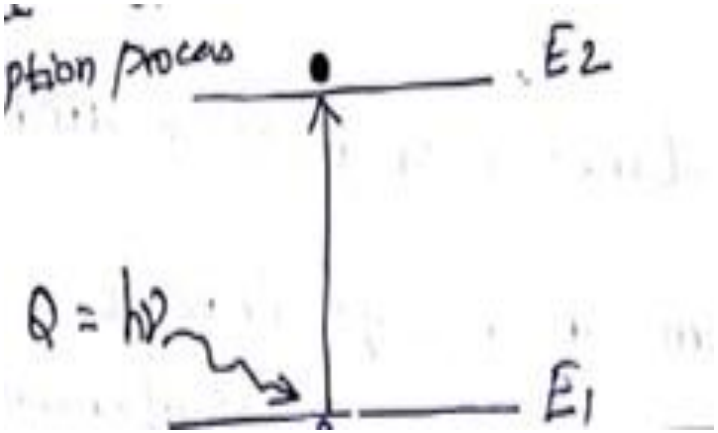
This leads to the increase of concentration of mobile charge carriers and increase the conductivity of the material.

So the material behaves as a photoconductor with a conductivity proptaional to photon flux, the effect is used to detect light.

Absorption:

- Let us consider two energy levels in semiconductor E_1 & E_2
- where E_1 corresponds to ground state

  E_2 corresponds to exited state
- At room temperature most of the electrons are in ground state
- When photons of energy grater or equal to bandgap incident on Semiconductor electron hole pairs are generated, this process is Called absorption



$$N_{ab} \propto QN_1 \Rightarrow N_{ab} = B_{12} Q N_1$$

N_{ab} number of atoms undergoing absorption process

N_1 number of atoms in E_1

Q energy density of incident radiation

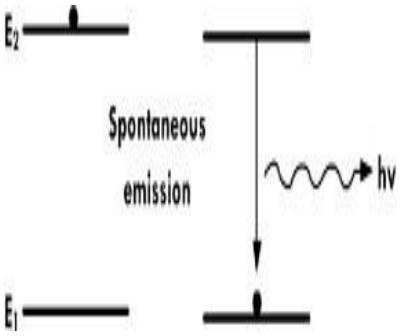
B_{12} proportionality constant

Emission process:

Generally the emission process are takes place in two types in optical devices

1. Spontaneous emission
2. Stimulated emission

Spontaneous emission: spontaneous emission, this process requires a conduction band energy state occupied by an electron and an empty valence band energy state. The electron Itself transit from conduction band to valence band spontaneously by releasing a photon.



This photon has a random direction and phase.

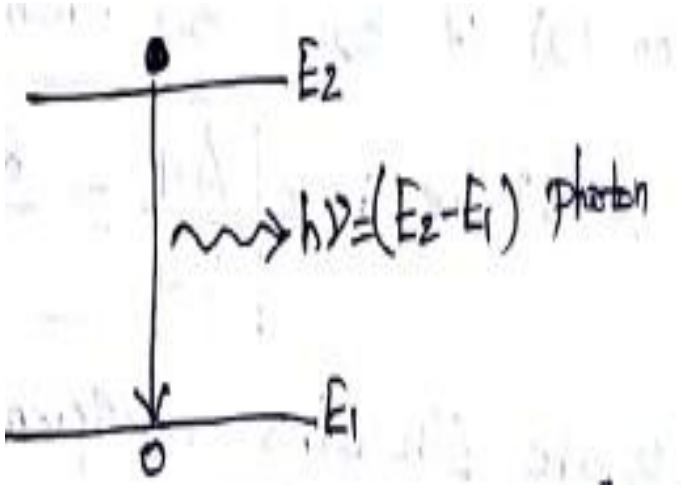
This is the opposite of the common situation in equilibrium, but at a finite temperature there will be a small number of full states in the conduction band and empty states in the valence band. Also, electrons and holes can be created via optical absorption and other pumping mechanisms.

Spontaneous emission:

➢When electron hole pairs are generated due to the absorption of incident radiation.

➢After a short time without any external stimulus the electron come back from unstable exited state (E_2) to ground state (E_1) by emitting a photon of energy

$$h\nu \geq E_2 - E_1$$



➢This process is called spontaneous emission

Then $N_{sp} \propto N_2 \Rightarrow N_{sp} = A_{21} N_2$

N_{sp} is the number of atoms undergoing spontaneous emission process

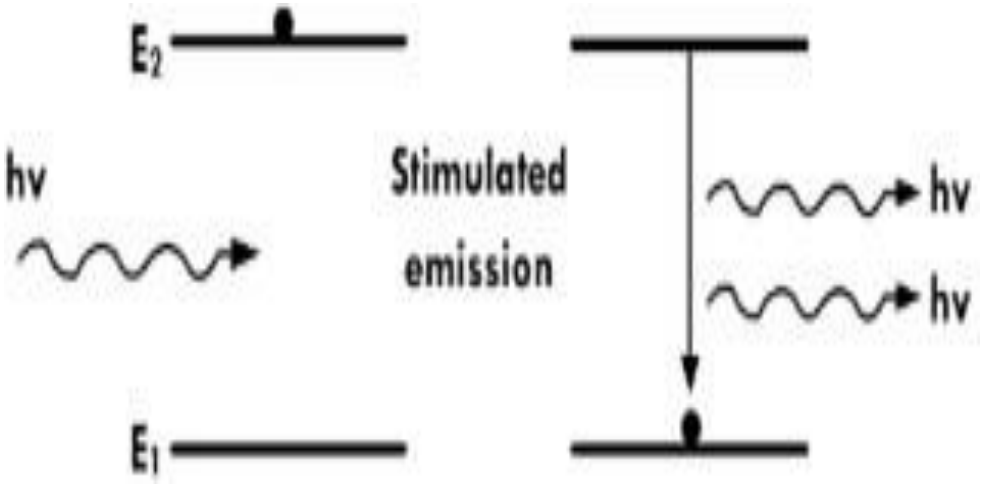
N_2 number of atoms in E_2

A_{21} proportionality constant

Stimulated emission:

- An incident photon causes an upper level atom to decay, emitting a "stimulated" photon whose properties are identical to those of the incident photon.

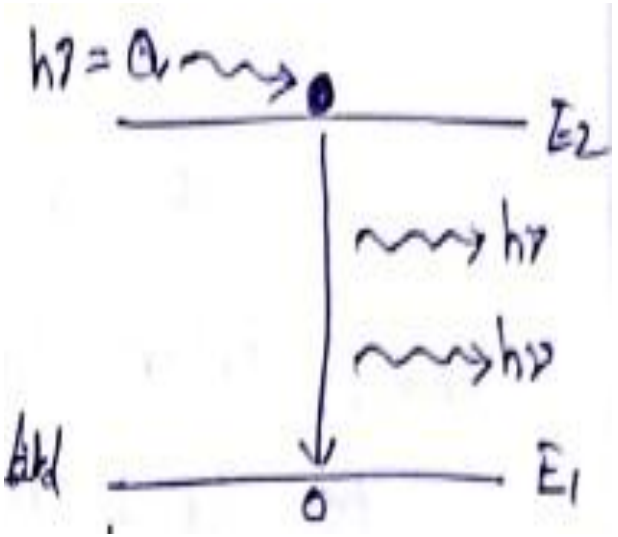
- The term "stimulated" underlines the fact that this kind of radiation only occurs if an incident photon is present



Stimulated emission:

➢If a photon of energy (hv) impinges on the electron which is presented in Exited state (E_2).

➢The electron stimulated back to the ground state by releasing the energy $hv \geq E_2\text{-}E_1$ which is in phase with the incident radiation. This process is called stimulated emission.



$$\mathbf{N_{st} = B_{21}\, Q\, N_2}$$

N_{st} number of atoms undergoing stimulated process

N_2 number of atoms in E_2

Q energy density of incident radiation

B_{21} proportionality constant

Ratio between Spontaneous and stimulated Coefficient

For a given system under equilibrium

Absorption = Emission (Spontaneous + stimulated)

$$N_1 Q B_{12} = N_2 A_{21} + N_2 Q B_{21}$$

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

From Boltzmann distribution law, at a given temperature (T), the ratio of population of two levels is given by

$$\frac{N_1}{N_2} = e^{(E_2 - E_1)/kT} = e^{h\nu/kT} \Rightarrow Q = \frac{A_{21}}{e^{h\nu/kT} B_{12} - B_{21}} \rightarrow (2)$$

Also, from planks body radiation theory

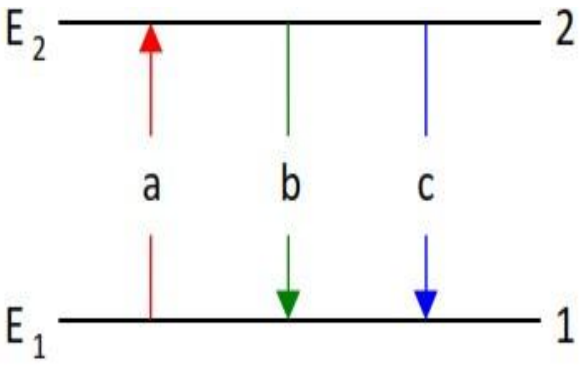
$$Q = \frac{8\pi hc}{\lambda^5} \times \left[\frac{1}{e^{h\nu/kT} - 1}\right] \rightarrow (3)$$

In equation (2) if $B_{21} = B_{12}$ then $Q = \frac{A_{21}}{B_{21}} \times \left[\frac{1}{e^{h\nu/kT} - 1}\right] \rightarrow (4)$

Comparing (3) & (4) we write $\boxed{\frac{A_{21}}{B_{21}} = \frac{8\pi hc}{\lambda^5}}$

Here A & B are Einstein Coefficients which gives value for ratio of Spontaneous and stimulated emission.

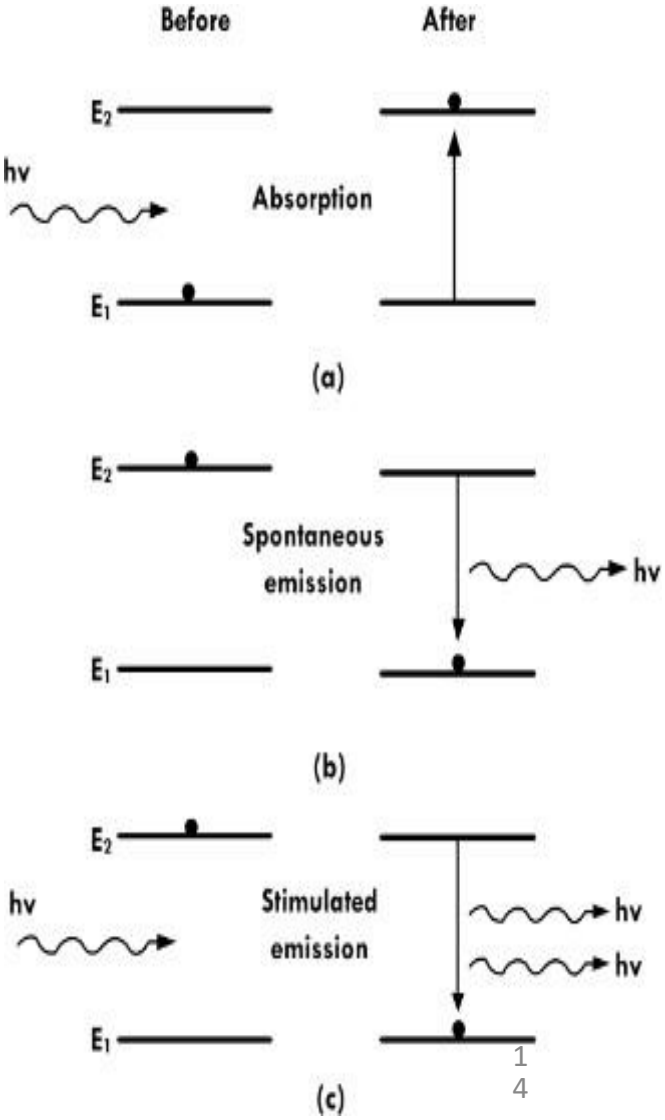
Overall picture of Absorption and emission processes



a absorption

b spontaneous emission

c stimulated emission



Absorption

Molecule absorbs a quantum of radiation (a photon) and is excited from 1 to 2.

$M + h\upsilon \rightarrow M^*$

(state 1) (state 2)

Spontaneous emission

M* (in state 2) spontaneously emits a photon of radiation.

$M^* \rightarrow M + h\upsilon$

Stimulated emission

A quantum of radiation is required to stimulate M* to go from 2 to 1.

$M^* + h\upsilon \rightarrow M + 2h\upsilon$

Recombination process:

- When a semiconductor is illuminated with light an electron in the valence band making an upward transition to conduction band.
- This results electron-hole pair generated, the reverse process of electron-hole annihilation is called recombination.
- Recombination process may be radiative or non- radiative

1. If electron annihilated with hole releases energy equal to $E \geq E_g$, it is called radiative recombination, in this process a photon of energy $E = h\nu$ is released
2. If electron annihilated with hole releases energy equal to $E < E_g$, it is called non-radiative recombination, in this process phonons are released

Recombination of electron – hole pairs is observed in different optical process

- **Luminescence:** Process where electron hole pairs created and recombined radiatively
- **Photoluminescence:** electron- hole pairs are generated due to absorption of light and recombination occurs radiatively
- **Cathodluminescence:** electron – hole pairs are generated by the electron bombardment and radiative recombination occurs
- **Electroluminescence:** process of radiative recombination following injection with pn-junction or similar device.

When a semiconductor is under equilibrium without any incident photon (or) injection of electron the carrier density can be calculated from an equilibrium Fermi level using Fermi Dirac statistics

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

But when light is illuminated non-equilibrium carrier concentration is created and above relation is not valid, hence Fermi Dirac distribution for electrons and holes in non-equilibrium condition are

$$f(E)_n \propto \exp\left(\frac{E_{Fn} - E_c}{kT}\right) \quad \text{for electrons}$$

$$f(E)_p \propto \exp\left(\frac{E_v - E_{Fp}}{kT}\right) \quad \text{for holes}$$

Further carrier concentration is calculated as

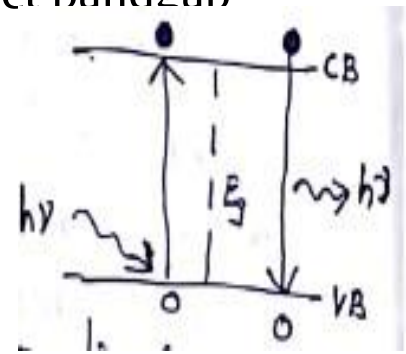
$$n = N_c \exp\left[\frac{E_{Fn} - E_c}{kT}\right] \quad \text{for electro}$$

$$p = N_v \exp\left[\frac{E_v - E_{Fp}}{kT}\right] \quad \text{for holes}$$

➢The excess carriers generated in semiconductor at non equilibrium condition must eventually recombine

Generation rate (G) = recombination rate (R)

➢The generation and recombination processes involve transition of charge carriers across the energy bandgap and is different for direct & indirect bandgap semiconductor materials.



➢The probability of radiative recombination is very high in direct bandgap semiconductors due to momentum & energy conservation

➢Recombintaion rate of charge carriers depends upon the lifetime of charge carriers

➢In general both radiative and noradiative recombinations are considered, the total life time is given as

$$\frac{1}{\tau} = \frac{1}{\tau_r} + \frac{1}{\tau_{nr}} \quad \text{where} \quad R = \frac{\Delta n}{\tau}$$

τ_r is radiative life time & τ_{nr} is non-radiative life time of charge carriers. Also total Recombination rate is given by

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

Internal quantum efficiency due to recombination Process is

$$\eta_r = \frac{1}{1+[\tau_r/\tau_{nr}]}$$

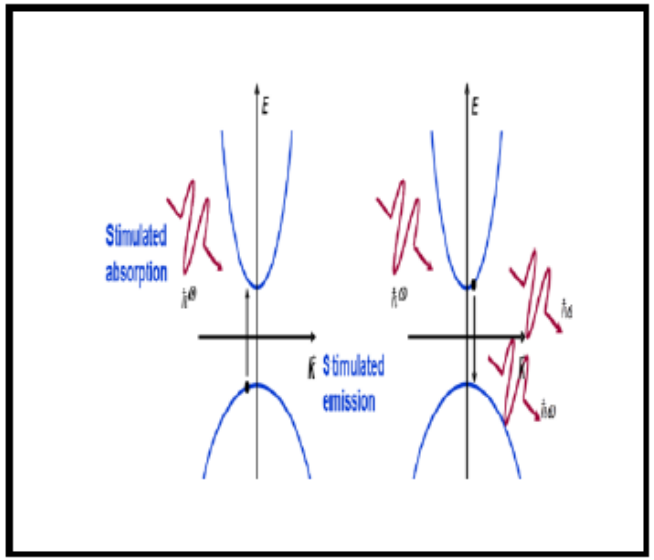
If τ_r/τ_{nr} is small in which τ_{nr} is large as possible, η_r increases leads to high radiative recombination in Semiconductor

Joint density of states

(Conservation of energy and momenta of electron when photon interacts)

Optical Joint Density of States

How many states are possible for photon interaction of energy hγ in valence and conduction band is given by optical joint density of states. To determine the density of state ργ with which a photon of energy hγ interacts under a condition of energy and momentum conservation in a direct band gap semiconductor.



To approximate this relation for a direct band-gap semiconductor by two parabolas,

$$E_2 = E_c + \frac{\hbar^2 K^2}{2m_c}$$

$$E_1 = E_v - \frac{\hbar^2 K^2}{2m_v}$$

$$h\gamma = E_2 - E_1$$

$$h\gamma = E_g + \frac{\hbar^2 K^2}{2m_v}$$

$$K^2 = \frac{2m_v}{\hbar^2}(h\gamma - E_g)$$

Here, substitute the value of K^2 in eq (1) & eq (2)

$$E_2 = E_c + \frac{m_v}{m_c}(h\gamma - E_g)$$

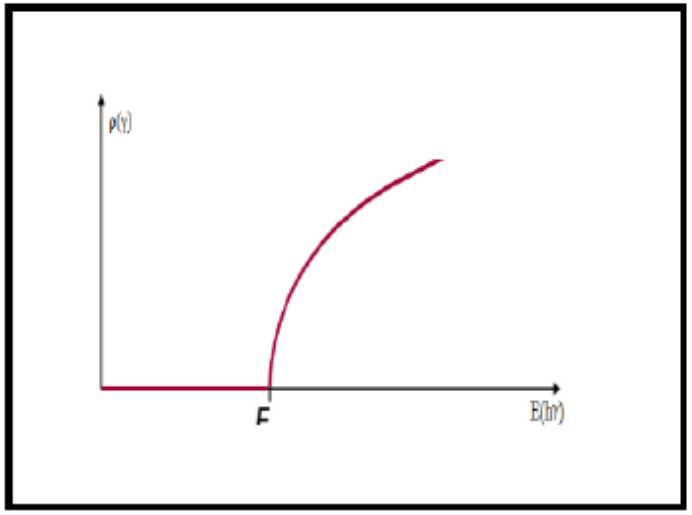
Similarly,

$$E_1 = E_v - \frac{m_v}{m_c}(h\gamma - E_g)$$

The one-to-one correspondence between E_2 and γ permits us to readily relative $\rho(\gamma)$ to the density of states $\rho_c(E_2)$ in conduction band by use of the incremental relation

$$\rho_c(E_2)dE = \rho(\gamma)\, d\gamma$$

Here $\rho_c(E_2)dE$ is no of states between E_2 *and* dE_2 and $\rho(\gamma)\, d\gamma$ is the number of states per unit volume of energy between $h\gamma$ and $h(\gamma+d\gamma)$ to interact.



Therefore,

$$\rho(\gamma) = \rho_c(E_2)\frac{dE}{d\gamma}$$

$$\rho(\gamma) = \frac{(2m_v)^{3/2}}{\pi\hbar^2}(h\gamma - E_g)^{1/2} \text{ for } h\gamma \geq E_g$$

The density of states which a photon of energy $h\gamma$ interact increases with $h\gamma \geq E_g$ in accordance with a square root law. Similarly One-to-One correspondence between E_1 and $\rho(\gamma)$ in equation, together with $\rho(\gamma)$ E_1, results in an expression for $\rho(\gamma)$ identical.

Density of States for Photons

To define the density of states for photons we assume that the photon is enclosed in a large cube of side length L, such that volume is $V= L^3$. The wave function of photon is a plane wave $e^{ik.\vec{r}}$ .We use the periodic boundary conditions that the wave function should be periodic in the x,y and z directions with a period L.

Because of the wave function has to be zero at boundaries. We have Quantization of wave number

$L.\ K = n2\pi$

$K_x = l\ \frac{2\pi}{L}$; $K_y = l\ \frac{2\pi}{m}$; $K_z = l\ \frac{2\pi}{n}$

The volume of state in K space is $(\frac{2\pi}{L})^3$

Density of States for Photons

Let us look at the integral using the number of states with a differential volume in the K-space.

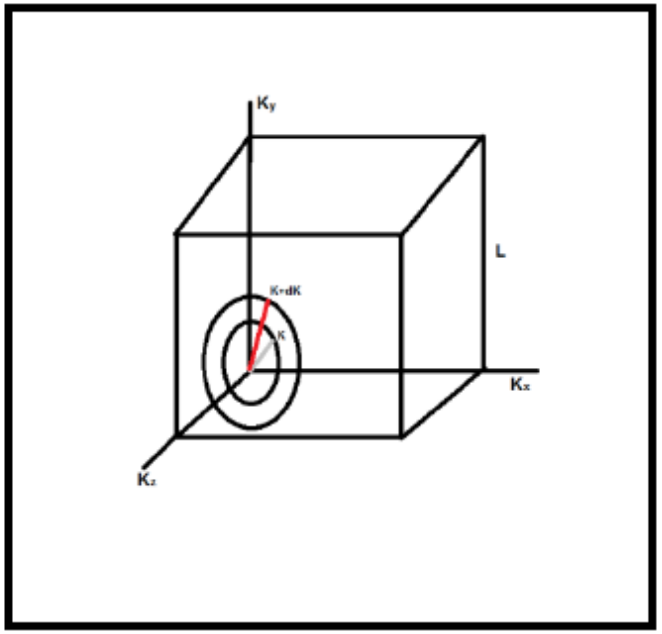
$$\frac{d^3K}{(\frac{2\pi}{L})^3} = \frac{K^2 dk d\Omega}{(\frac{2\pi}{L})^3}$$

Where $d\Omega$ is the differential solid angle.

Therefore

$$N(E_{21}) = \frac{2}{V}\sum_{K}\delta\ (E_2 - E_1 - E_k)$$

$$N(E_{21}) = 2\int \frac{K^2 dk d\Omega}{(2\pi)^3}\delta\ (E_2 - E_1 - E_k)$$



$$E_k = \hbar\omega_k = \frac{\hbar KC}{n_r}$$

Where, C/n_r is the speed of light in medium with refractive index of n_r. Here integration over solid angle is 4π.

Density of States for Photons

$$K = \frac{E_k n_r}{\hbar C}$$

$$dK = \frac{n_r 2\pi}{hC} dE_k$$

$$N(E_{21}) = 2 \int \frac{K^2 dk d\Omega}{(2\pi)^3} \delta\ (E_{21} - E_k)$$

$$N(E_{21}) = 2 \int \frac{K^2}{(2\pi)^3} \frac{n_r 2\pi}{hC}\ dE_k\ (4\pi) \delta\ (E_{21} - E_k)$$

$$N(E_{21}) = 2 \int \frac{1}{(2\pi)^3} \left(\frac{E_k n_r 2\pi}{hC}\right)^2 \frac{n_r 2\pi}{hC}\ dE_k (4\pi)\ \delta\ (E_{21} - E_k)$$

$$N(E_{21}) = \frac{2 \times 4\pi \times (2\pi)^3 (n_r)^3}{(2\pi)^3 (hC)^3} \int (E_k)^3\ dE_k\ \delta\ (E_{21} - E_k)$$

$$N(E_{21}) = \frac{8\pi (n_r)^3}{(hC)^3} E_{21}^2 \quad [\hbar = \frac{h}{2\pi}; h = \hbar\, 2\pi]$$

$$N(E_{21}) = \frac{8\pi E_{21}^2 (n_r)^3}{8\pi^3 \hbar^3 C^3} = \frac{E_{21}^2 (n_r)^3}{\pi^2 \hbar^3 C^3}$$

Which is the number of states with photon energy E_{21} per unit volume per energy interval.

DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

Optical Transitions Using Fermi's Golden Rule

Fermi's Golden Rule

Introduction

Fermi's golden rule is a simple expression for the transition probabilities between states of a quantum system, which are subjected to a perturbation. It is used for a large variety of physical systems covering, e.g., nuclear reactions, optical transitions, or scattering of electrons in solids.

Consider a semiconductor illuminated by electromagnetic radiations (light). The interaction between photons and the electrons in the semiconductor can be described by the Hamiltonian operator.

$$\vec{H} = \frac{1}{2m_0}(\vec{p} - e\vec{A})^2 + \overrightarrow{V}(r)$$

Where ,

m_0 *is the free electron mass,* $\vec{A}$ *is the vector potential accounting part of electromagnetic field.*

$\overrightarrow{V}(r)$ *is the periodic potential and* $e = -|e|$

Optical Transitions Using Fermi's Golden Rule

In general Transition probability for Fermi's golden rule

$$\lambda_{if} = \frac{2\pi}{\hbar} |M_{if}|^2 Pf$$

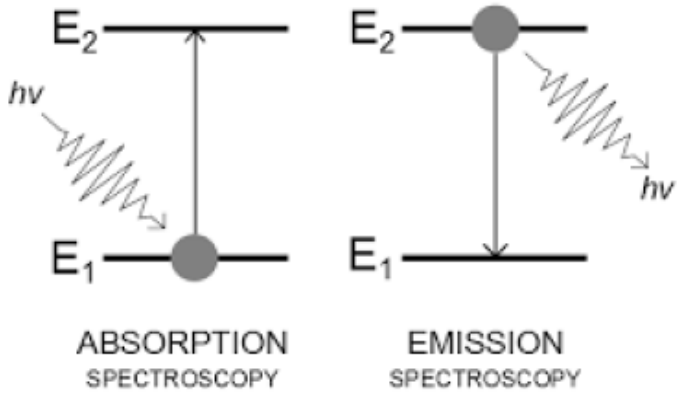
Where, $|M_{if}|^2$ - is Matrix element for interaction $|M_{if}|^2 = |< b|H'(r)|a >|^2$ and,

Pf – is the number of continuum state per unit volume or density of final state.

$(Pf = \delta (E_b - E_a - \hbar\omega)$.

Where $E_b > E_a$ has been assumed. The total upward transition rate per unit volume(S^{-1}, cm^{-3}) in the crystal taking into account the probability that state a is occupied and state b is empty is

Transition Rate due to electron-photon interaction



Using the time dependent perturbation theory, the transition rate for the absorption of a photon can be derived, assuming an electron is initially at state E_1 is given by Fermi's Golden rule

$$W_{abs} = \frac{2\pi}{\hbar} |< b|H'(r)|a >|^2 \, \delta\,(E_b - E_a - \hbar\omega)$$

Where $E_b > E_a$ is assumed.

The total upward transition rate per unit volume

$$R_{a-b} = \frac{2}{V} \sum_{K_a} \sum_{K_b} \frac{2\pi}{\hbar} |H'_{ba}|^2 \, \delta\,(E_b - E_a - \hbar\omega) f_a\,(1 - f_b)$$

Transition Rate due to electron-photon interaction

Where we sum over the initial and final states and assume that the Fermi-Dirac distribution f_a is the probability that the state a is occupied. A similar expression holds for f_b with E_a replaced by E_b, and $(1 - f_b)$ is probability that the state b is empty. The prefactor 2 takes into account the sum over spins, and the matrix element H'_{ba} is given by

$$H'_{ba} = |< b|H'(r)|a >|^2 = \int \psi^*(r) H'(r) \psi_a(r) d^3r$$

Similarly, The transition rate for the emission of a photon (fig.2) if an electron is initially at state b is.

$$W_{ems} = \frac{2\pi}{\hbar} |< a|H'^{+}(r)|b >|^2 \delta(E_a - E_b + \hbar\omega)$$

The downward transition rate per unit volume (S^{-1} cm^{-3}) is

$$R_{b-a} = \frac{2}{V} \sum_{K_a} \sum_{K_b} \frac{2\pi}{\hbar} |H'^{+}_{ab}|^2 \delta(E_a - E_b + \hbar\omega) f_b (1 - f_a)$$

Transition Rate due to electron-photon interaction

Using the even property of the delta function, $\delta(-x) = \delta(x) and \ |H'_{ba}| = |H'^{+}_{ab}|$.

The net upward transition rate per unit volume can be written as,

$$R = R_{a\to b} - R_{b\to a}$$

$$R = \frac{2}{V}\sum_{K_a}\sum_{K_b}\frac{2\pi}{\hbar}|H'_{ba}|^2\,\delta(E_b - E_a - \hbar\omega)(f_a - f_b)$$

An Optical absorption coefficient

The absorption coefficient α_0 $(\frac{1}{Cm})$ in the crystal is the fraction of photons absorbed per unit distance

$$\alpha_0 = \frac{Number\ or\ Photons\ absorbed\ per\ second\ per\ unit\ volume}{Number\ of\ injected\ photons\ per\ second\ per\ unit\ area}$$

The injected number of photons per second per unit area of the optical intensity ρ (W/Cm^2) divided by the energy of a photon (ħω). Therefore,

$$\alpha(\hbar\omega) = \frac{R}{\frac{p}{\hbar\omega}} = \frac{\hbar\omega R}{\left(\frac{n_r C \varepsilon_0 \omega^2 {A_0}^2}{2}\right)}$$

Where, R is the net upward transition rate per unit volume

ω - $\frac{2\pi}{\lambda}$, wave number / angular velocity

C- Velocity of light

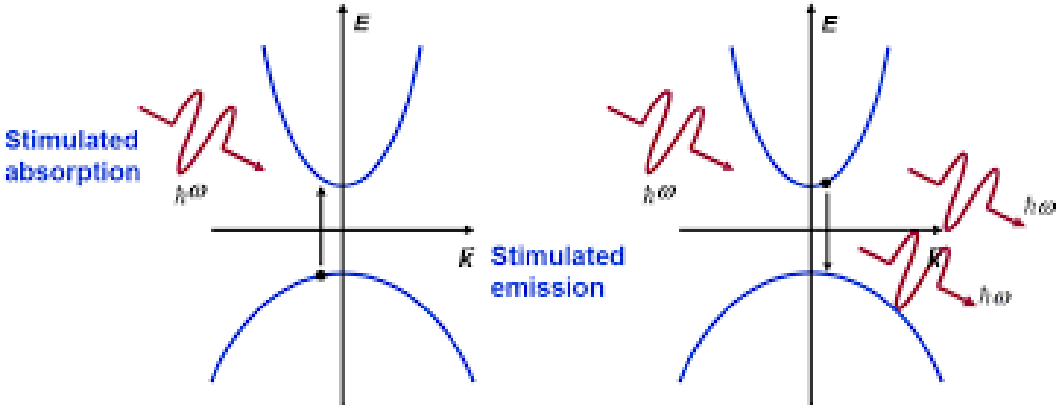
n_r – Refractive index of the medium.

A – Vector potential for electromagnetic field.

ε_0- Permittivity of the free space.

Optical Gain and Loss in semiconductor

Optical Gain in semiconductor defines the stimulated emission associated with light emission created by recombination of electrons and holes.



Optical Loss in semiconductor defines the stimulated absorption associated with light absorption created by generation of electrons and holes.

In a semiconductor crystal, consider an electron initially occupies a single state and makes a transition to one of a large number of final states due to photon interaction.

The electron-photon interactions in the crystal is characterized by Fermi's Golden Rule and gives the transition rate for a single pair of conduction and valence band states.

Each downward transition generates one photon and upward transition absorbs one photon.

$W_{c \rightarrow v}$ is the downward transition rate and $W_{v \rightarrow v}$ is the upward transition rate which can be find using Fermi Golden rule

$$W_{c\to v} = \frac{2\pi}{\hbar}\left|H'_{eh}\right|^2 \rho_{red} f_c (1-f_v)$$

$$W_{v\to c} = \frac{2\pi}{\hbar}\left|H'_{eh}\right|^2 \rho_{red} f_v (1-f_c)$$

Where H' is time dependent perturbation to the original Hamiltonian, It is to induce electronic transition between conduction and valence band. f_v and f_c the Fermi distribution and ρ_{red} is reduced density of state.

Explanation for Optical Gain

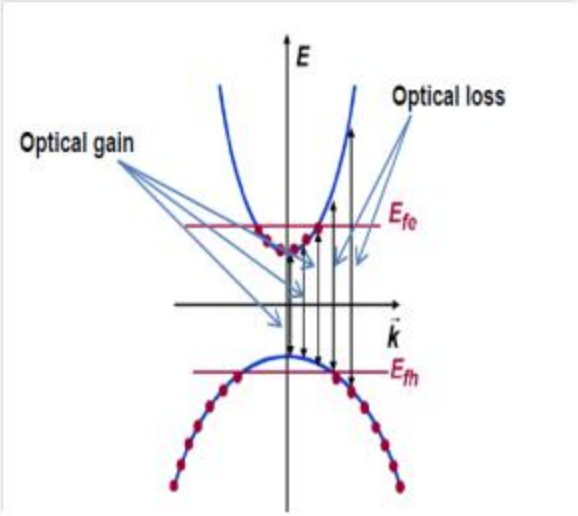
Optical gain in semiconductor is caused by photon-induced transitions of electrons from the conduction band to the valence band

Optical gain in the material is attained when we inject a carrier density beyond N_{tr} such that the quasi-Fermi levels are separated by an energy greater than the band gap.

If the number of downward transition per seconds exceeds the number of upward transition, there will be a net generation of photons, and optical gain can be achieved.

Optical Gain in Semiconductor

Each downward transition generator a new photon while upward absorbs one. If the number of downward transition for seconds exceeds the number of upward transition there will be a net generation of photons and optical gain can be achieved. The condition for optical gain is net stimulated emission is greater than absorption process.



The optical gain is given as $(g) = \frac{1}{\phi}\left(\frac{d\phi}{dz}\right)$

Where,

ϕ is the photon flux (the number of photons per cross section area unit in the unit of time)

z is the direction of the electromagnetic field propagation,

$$\frac{d\Phi}{dz} = W_{C\to V} - W_{V\to C}$$

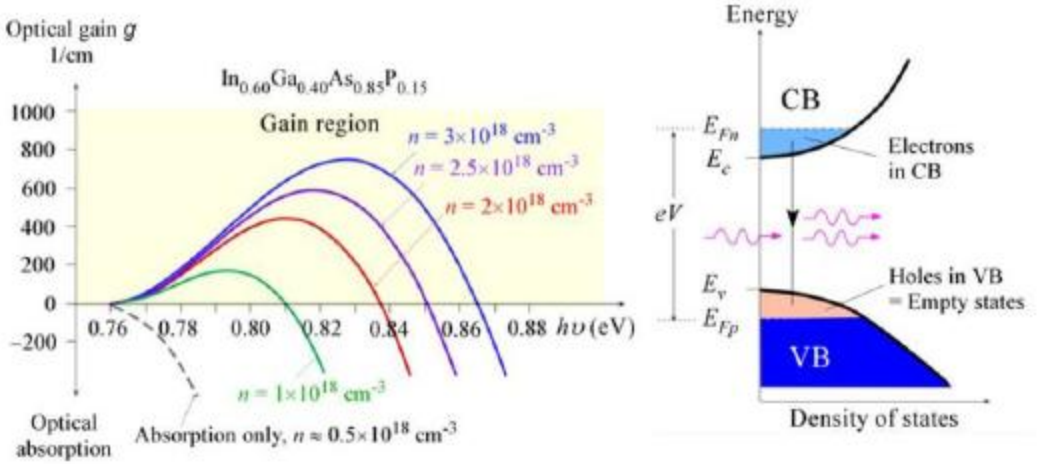
Optical Gain in Semiconductor

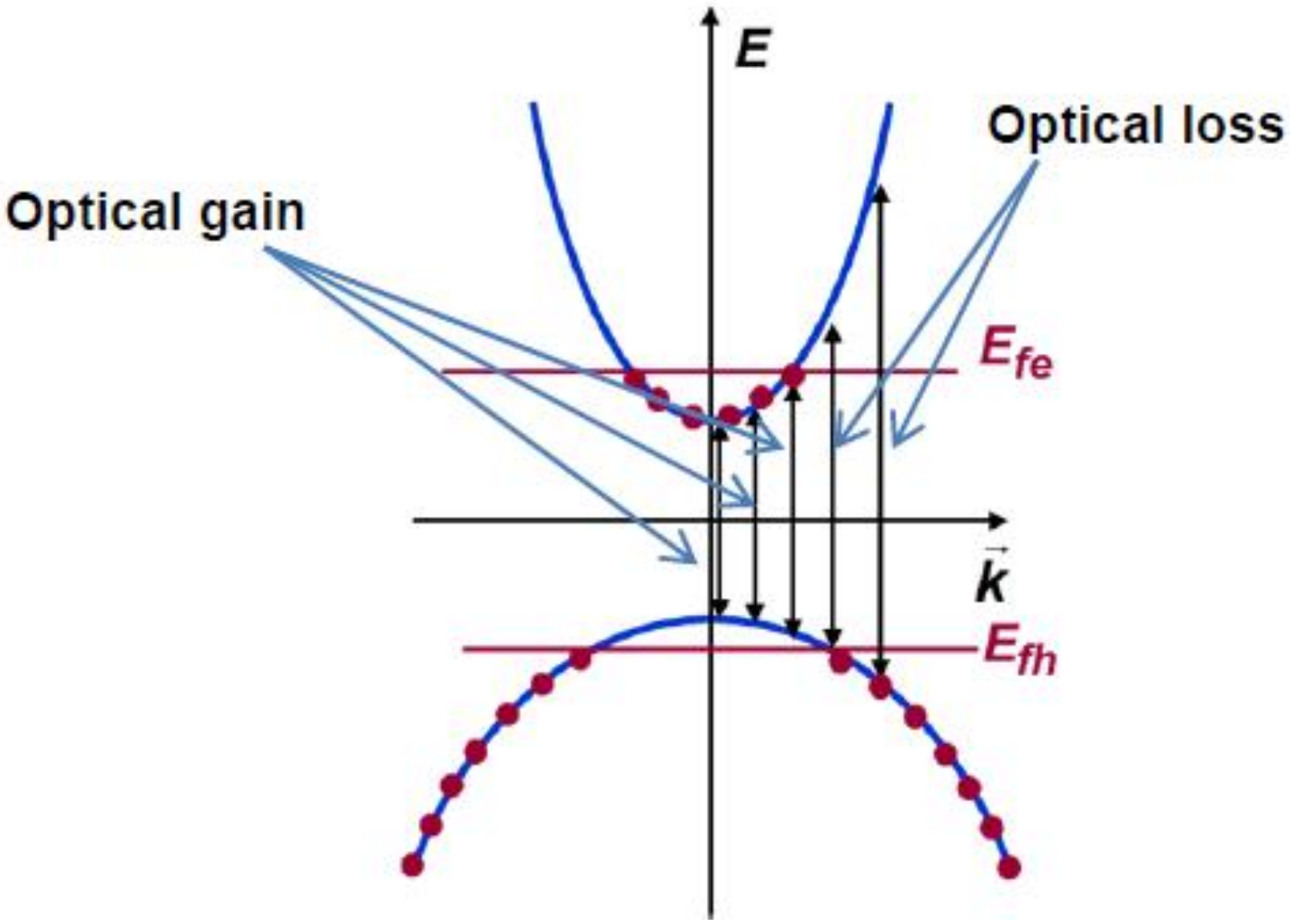
So the resultant gain we explained as

$$g = \frac{1}{\varphi} \cdot \frac{2}{V} \sum_{K_a} \sum_{K_b} \frac{2\pi}{\hbar} \left| H'_{ba} \right|^2 \delta \left(E_a - E_{ab} + \hbar\omega \right) (f_b - f_a)$$

The gain and absorption (Loss) profiles as a function of energy is shown in Fig.

Optical Gain Curve




E
Optical loss
Optical gain
E_{fe}
$\vec{k}$
E_{fh}

The optical gain experienced by an incoming photon is very much dependent on the photon's energy.

From the figure, Given a value for the Fermi level splitting, optical frequencies for which $E_g < \hbar\omega < E_{fe}\text{-}E_{fh}$ experience optical gain

The condition $E_g < \hbar\omega < E_{fe}\text{-}E_{fh}$ is the condition for population inversion and can be realized if, for example, electrons are removed from the valence band and placed in the conduction band.

Explanation for Optical Loss

Optical loss in semiconductor is caused by photon-induced transitions of electrons from the valence band to the conduction band

If the number of upward transition per seconds exceeds the number of downward transition, there will be a net absorption of photons, and optical loss can be achieved.

The light loss coefficient α(ω) for optical gain is less than zero or negative

The light loss coefficient α(ω) for optical gain is greater than zero or positive