

Semiconductor Physics and Computational Methods (21PYB102J)

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**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

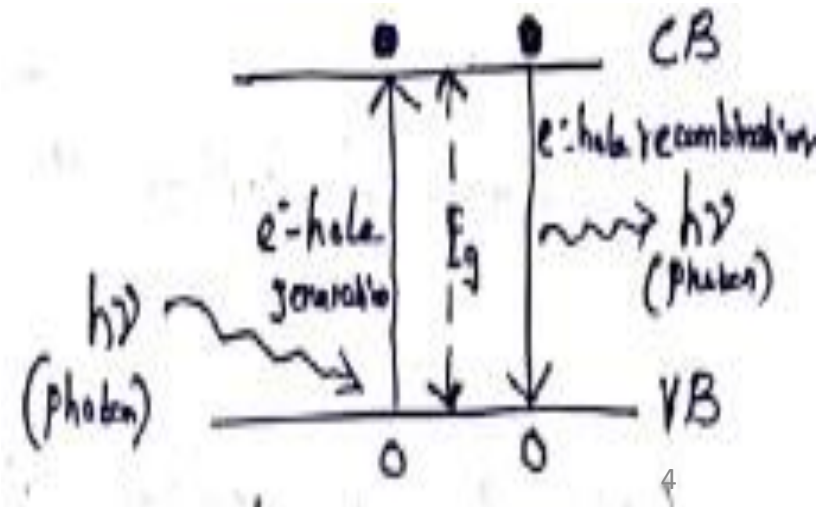
- 1. Band to band transition (Inter band transition)**
- 2. Impurity level to band transition**
- 3. Free carrier transition (Intra band transition)**

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

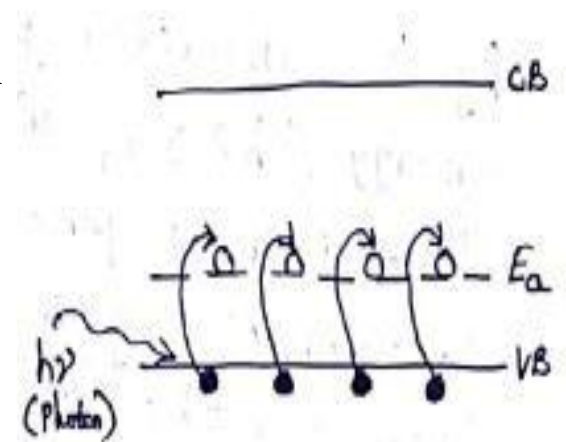
Eg: Band to Band transition in GaAs can results absorption and emission of photons with wavelength of $0.87 \mu\text{m}$ or ($E_g = 1.42 \text{ eV}$)



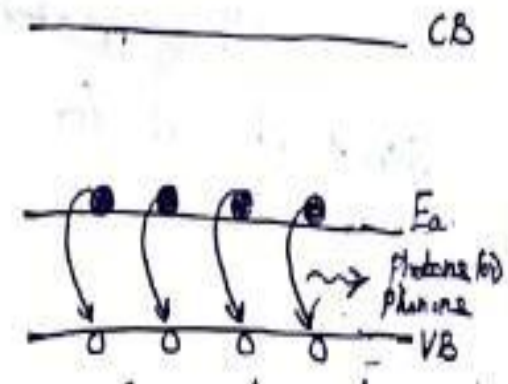
2. Impurity level to band transition:

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 $14 \mu\text{m}$

3. Free carrier transition (Intra band transition):

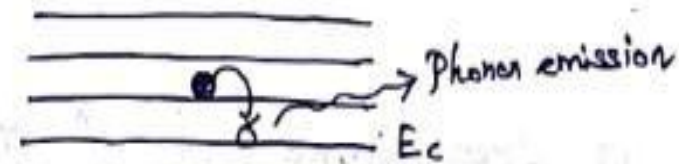
An absorbed photon can impart its energy to an electron in a given band, causing it to move to higher level in that band.

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.



Photon - (Absorption Process)



Phonon - (Recombination process)

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.

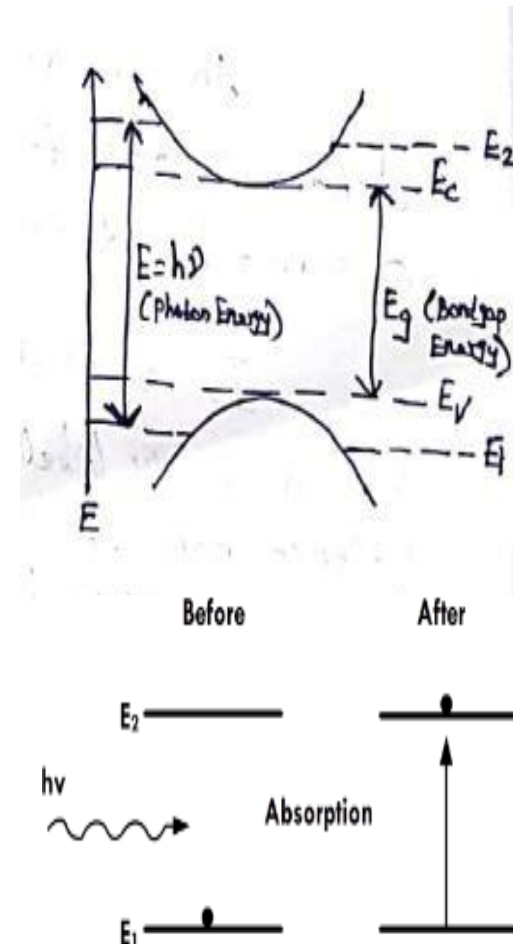
Consider direct band to band absorption:

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 excited state

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

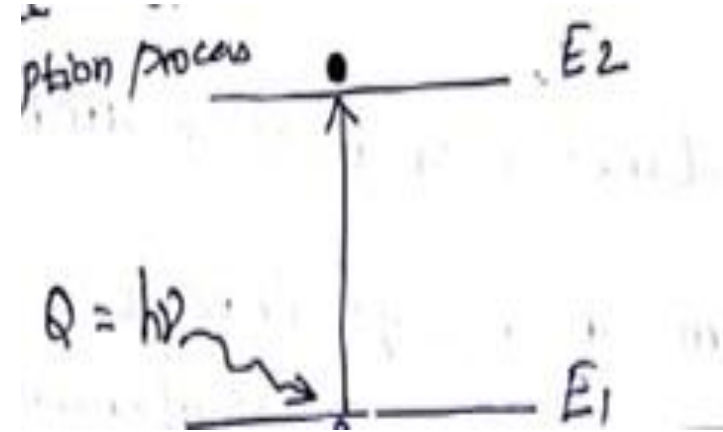
$$N_{ab} \propto QN_1 \Rightarrow N_{ab} = B_{12} Q N_1$$

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

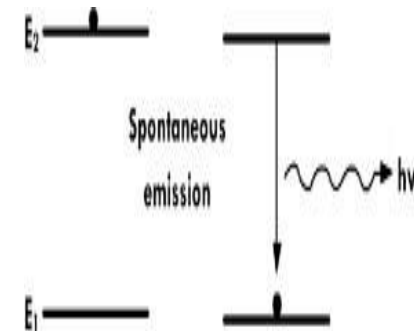


Emission process:

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 excited state (E_2) to ground state (E_1) by emitting a photon of energy

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

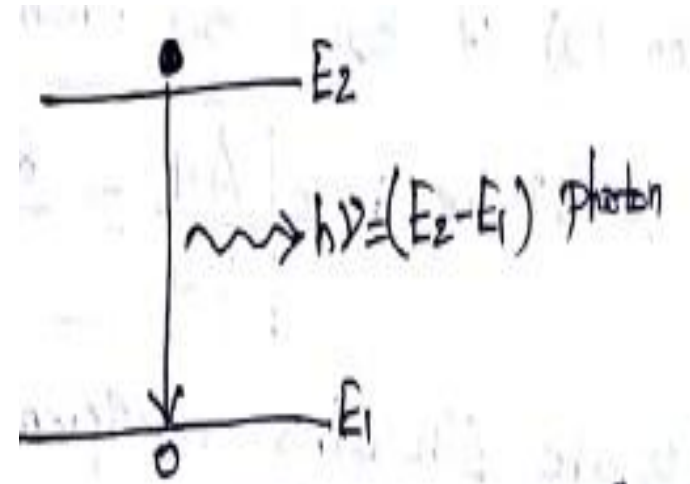
➤ This process is called spontaneous emission

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

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

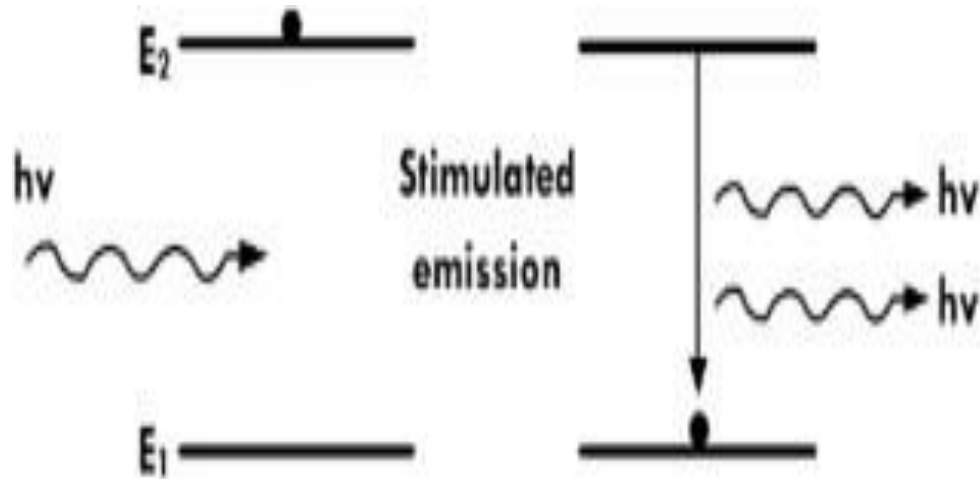
N_2 number of atoms in E_2

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 ($h\nu$) impinges on the electron which is presented in Excited state (E_2).

➤ The electron stimulated back to the ground state by releasing the energy $h\nu \geq E_2 - E_1$ which is in phase with the incident radiation. This process is called stimulated emission.

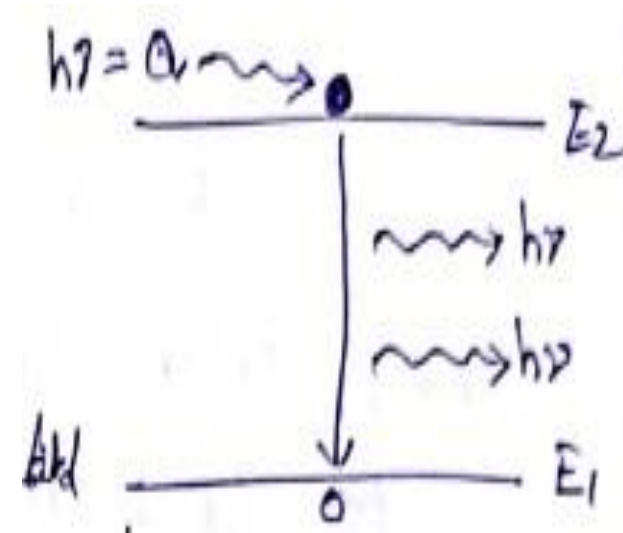
$$N_{st} = B_{21} Q N_2$$

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

$$\text{Absorption} = \text{Emission (Spontaneous + Stimulated)}$$

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

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

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 Planck's body radiation theory

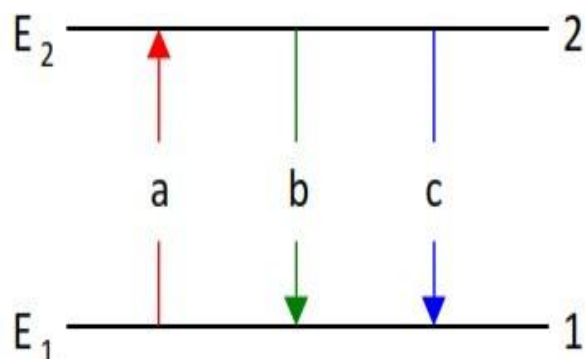
$$Q = \frac{8\pi h c}{\lambda^5} \times \left[\frac{1}{e^{h\nu/kT} - 1} \right] \rightarrow (3)$$

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

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

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

Overall picture of Absorption and emission processes



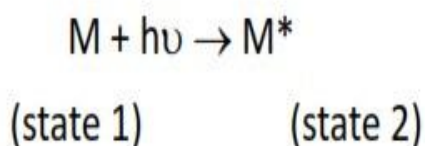
a **absorption**

b **spontaneous emission**

c **stimulated emission**

Absorption

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



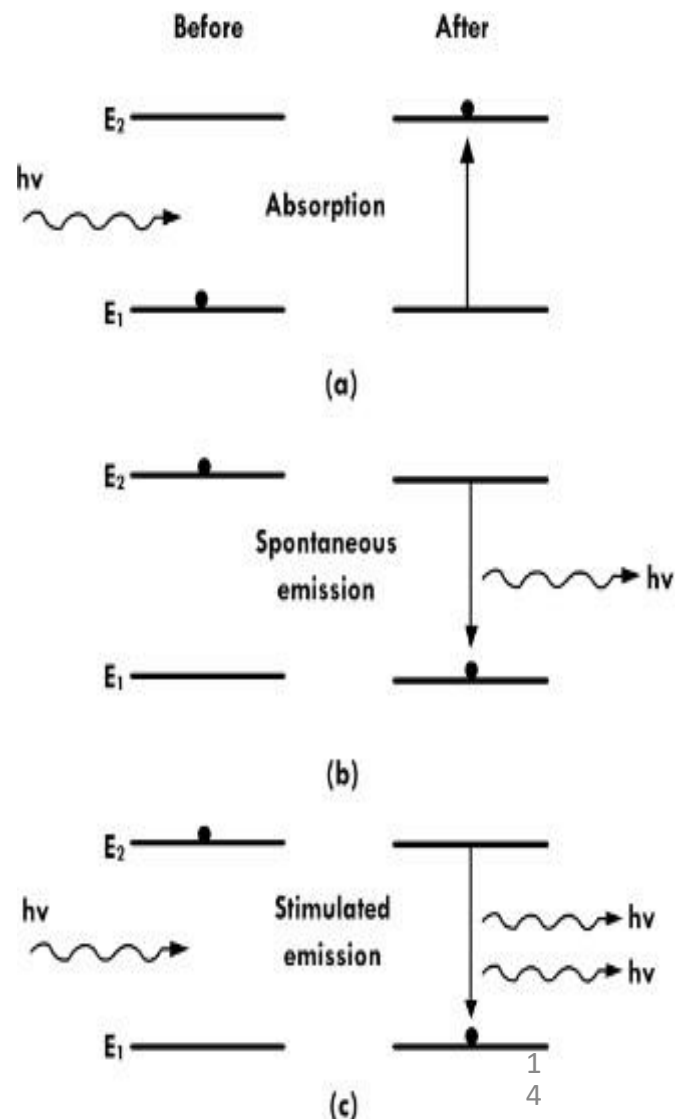
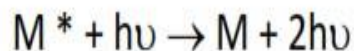
Spontaneous emission

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



Stimulated emission

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



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

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

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

Further carrier concentration is calculated as

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

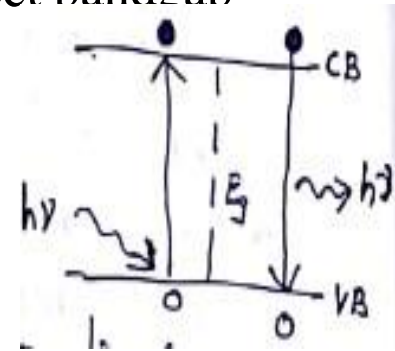
$$p = N_v \exp\left[\frac{E_v - E_{Fp}}{kT}\right] \text{ for holes}$$

➤ 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



➤ Recombination rate of charge carriers depends upon the lifetime of charge carriers

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

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

where

$$R = \frac{\Delta n}{\tau}$$

τ_r is radiative lifetime & 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

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Session – 7 MODULE-III

Optical Joint Density of States

Introduction:

- We have density of states for electrons in the conduction band (CB) and density of states for holes in the valence band (VB).
- Whole concentration depends on the density of the states in the valence band but in photon interactions, you have one state in the VB and one in the CB and therefore, we define an optical joint density of states
- Optical processes, such as emission and absorption involve the energy states in the valence band and the energy states in the conduction band.
- **Therefore, it is important to know how many states are available for a photon of energy ($h\nu$) to interact with.**
- **Optical joint density of states simultaneously takes care of number of states in both valence band and conduction band for a given energy ($h\nu$) of photon.**
- **Optical joint density of states tells us the number of states available for photons to interact simultaneously in the valence band and the conduction band.**
- In all optical processes, it is the joint density of states which is important.

Derivation:

- We know that density of states defines the number of allowed energy states per unit volume.
- To know or find the number of transitions or emissions (because that gives the no. of photons emitted) we need to know the emissions per unit volume. This can also give an idea of the power emitted.
- The number of emissions per unit volume can be found by multiplying density of states and probability of occupations.
- Concentration of electrons in conduction band is given by:

$$n_e = f(E) \cdot \int Z_c(E) \cdot dE$$

- Concentration of holes in valance band is given by:

$$n_h = [1 - f(E)] \cdot \int Z_v(E) \cdot dE$$



Derivation:

- Suppose a radiation of energy $h\nu$ is incident on an electron sitting at certain level in valence band (E_1), it makes a transition to a vacant state in conduction band (E_2).
- This means that absorption involves a certain energy level in valence and a corresponding vacant level in conduction band.
- Similarly, if there is an electron at certain energy level (E_2') in conduction band and it makes a transition at a vacant level (E_1') in valence band, a photon with energy $h\nu'$ is emitted.
- We can thus say that absorption and emission involve a state in valence band and conduction band.
- For a fixed incident energy $h\nu$, if E_2 is fixed then E_1 will also be fixed.
- For a given energy $h\nu$ there are several pairs of $E_2 - E_1$ and so there are number of pairs of states available for a photon of energy $h\nu$ to interact and this is given by density of states.

Derivation:

- Since the absorption or emission takes place from the top of valence band and bottom of conduction band respectively, we can have a parabolic approximation for any level in conduction and valence band respectively.

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

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

- The energy of photon $h\nu$ is given by:

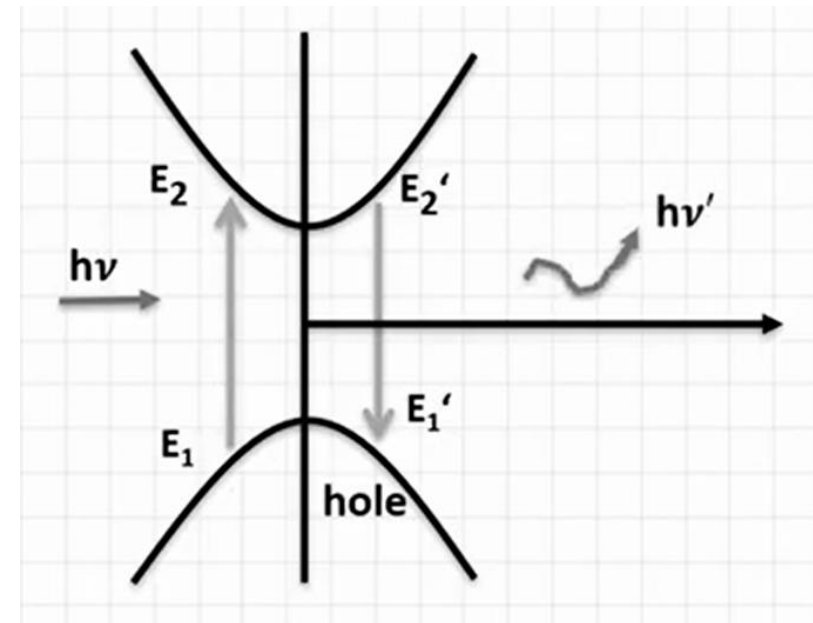
$$h\nu = E_2 - E_1$$

$$\Rightarrow h\nu = \left(E_c + \frac{\hbar^2 k^2}{2 m_c} \right) - \left(E_v - \frac{\hbar^2 k^2}{2 m_v} \right)$$

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

$$\Rightarrow h\nu = E_g + \frac{\hbar^2 k^2}{2} \left(\frac{1}{m_r} \right)$$

$$\Rightarrow k^2 = (h\nu - E_g) \frac{2 m_r}{\hbar^2} \dots\dots\dots (3)$$



Optical Joint density of states



Derivation:

$$E_1 = E_v - \frac{\hbar^2}{2m_v} (h\nu - E_g) \frac{2m_r}{\hbar^2}$$

$$\Rightarrow E_1 = E_v - \frac{m_r}{m_v} (h\nu - E_g) \dots\dots\dots (5)$$

- There is one to one correspondence between ' E_1 ' and ' ν '
- Hence, We have,

$$Z_c (E_2) dE_2 = Z (\nu) d\nu \dots\dots\dots (6)$$

- Where, $Z(\nu)d\nu$ is the number of states per unit volume available for photons of energy between $h\nu$ and $h(\nu+d\nu)$ to interact (either absorb or emit).
- Once we find out $Z(\nu)d\nu$, i.e. density of states available for interaction and multiply it by probability of emission or absorption, we can obtain total number of emission or absorption per unit volume.
- From equation (6),

$$Z (\nu) = Z_c (E_2) \frac{dE_2}{d\nu} \dots\dots\dots (7)$$

Derivation:

➤ From equations (1) & (3),

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

$$\Rightarrow (E_2 - E_c)^{\frac{1}{2}} = \left(\frac{m_r}{m_c} \right)^{\frac{1}{2}} (h\nu - E_g)^{\frac{1}{2}} \dots\dots\dots (8)$$

➤ From equation (7), We have

$$Z(\nu) = \frac{1}{2\pi^2} \left(\frac{2m_c}{\hbar^2} \right)^{\frac{3}{2}} (E_2 - E_c)^{\frac{1}{2}} \cdot h \cdot \frac{m_r}{m_c}$$

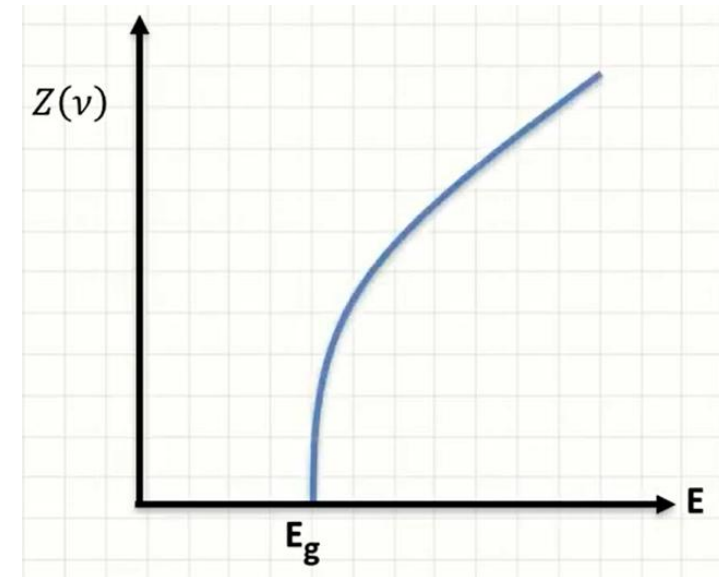
➤ Substituting value of $(E_2 - E_c)^{1/2}$

➤ From equation (8)

$$\Rightarrow Z(\nu) = \frac{1}{2\pi^2} \left(\frac{2m_c}{\hbar^2} \right)^{\frac{3}{2}} \cdot h \cdot \frac{m_r}{m_c} \cdot \left(\frac{m_r}{m_c} \right)^{\frac{1}{2}} (h\nu - E_g)^{\frac{1}{2}}$$

$$\Rightarrow Z(\nu) = \frac{1}{\pi \hbar^2} (2m_r)^{\frac{3}{2}} \cdot (h\nu - E_g)^{\frac{1}{2}} \dots\dots\dots (9)$$

➤ This is expression for optical joint density of states.



Optical joint density of states vs. Photon Energy ($h\nu$)

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Session – 7 MODULE-III

Density of States for Photons

Introduction:

- Quanta of the electromagnetic radiation are called photons
 - Properties of photons
 - Mass = 0
 - Charge = 0
 - Energy = $h\nu = \hbar\omega$
 - Momentum = $\hbar k$
- **Density of states for photons is the total number of allowed states per unit volume in the energy range of E and E+dE.**

Derivation::

➤ Density of states $g(E) = \frac{1}{V} \frac{dN(E)}{dE}$

- Where 'N(E)' is the total number of states from 0 to E.
- Analogous to our previous discussion in 'n' space, we can calculate the density of states by counting states in k-space by integrating over a volume.
- Each state is specified by three quantum numbers that represent a point on a cubic grid defined by the k_x , k_y , k_z dimensions.
- Allowed values of 'k' form a regular grid of points in k-space

$$k_i = \frac{2\pi}{L_i} m_i \quad m_i = 0, \pm 1, \pm 2 \dots \quad k^2 = k_x^2 + k_y^2 + k_z^2$$

- The total number of states below a given 'k' can be determined by integrating over a sphere with radius 'k' to obtain the k-space volume, and dividing by the volume of a single state.

Derivation::

Volume of the sphere in k – space with radius ' k ' is $= \frac{4}{3} \pi k^3$

Volume of a single state in k – space $= \left(\frac{2\pi}{L} \right)^3 = \frac{8\pi^3}{L^3} = \frac{8\pi^3}{V}$

Total number of states $N(E) = \frac{\left(\frac{4}{3} \pi k^3 \right)}{\left(\frac{8\pi^3}{V} \right)} = \frac{V}{6\pi^2} k^3$

$$\frac{dN(E)}{dE} = \frac{V}{2\pi^2} k^2 \frac{dk}{dE}$$

Density of states $g(E)$ $= \frac{1}{V} \frac{dN(E)}{dE} = \frac{1}{2\pi^2} k^2 \frac{dk}{dE}$

Density of States for Photons



Derivation:

For photons, Energy (E) = $\hbar\omega = \hbar(ck)$

$$\frac{dk}{dE} = \frac{1}{\hbar c}$$

where 'c' is the speed of light

$$\text{Density of states } g(E) = \frac{1}{2\pi^2} k^2 \frac{dk}{dE} = \frac{1}{2\pi^2} \left(\frac{E}{\hbar c}\right)^2 \left(\frac{1}{\hbar c}\right)$$

$$\text{Density of states } g(E) = \frac{1}{2\pi^2} \left(\frac{1}{\hbar c}\right)^3 E^2$$

We need to multiply the above equation by 2 since there are two (transverse) polarization states of the photon,

$$\text{Density of states of photons } g(E) = \frac{1}{\pi^2} \left(\frac{1}{\hbar c}\right)^3 E^2$$

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**Session – 8
MODULE-III**

**Fermi's Golden Rule
Transition Rate due to electron-photon interaction**



Introduction:

- It is also referred to as the “**Golden Rule of time-dependent perturbation theory**”.
- Fermi's golden rule is a simple expression for the transition probabilities between states of a quantum system, which are subjected to a perturbation.
- Fermi's Golden Rule provides the rate at which atomic or electronic transitions take place between two states.
- The rates are calculated from probabilities determined by transition matrix elements in quantum mechanical, first-order perturbation theory.
- It applies to a wide range of optical and electronic processes for which the initial and final states can be described by wave functions.

Fermi's Golden Rule



- The transition probability is of the general form:

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

Transition probability *Matrix element for the interaction* *Density of final states*

- A transition will proceed more rapidly if the coupling between the initial and final states is stronger.
- This coupling term is traditionally called the “**matrix element**” for the transition.
- The matrix element can be placed in the form of an integral where the interaction which causes the transition is expressed as a potential ‘**V**’ which operates on the initial state wave function.

$$M_{if} = \int \Psi_f^* V \Psi_i dv$$

Wavefunction for final state *Wavefunction for initial state*
Operator for the physical interaction which couples the initial and final states of the system.

Optical Transitions using Fermi's Golden Rule:

$$\text{Transition Probability } \lambda_{if} = \frac{2\pi}{\hbar} |M_{if}|^2 \rho_f$$

$$|M_{if}|^2 = |\langle b | H'(r) | a \rangle|^2$$

$$\rho_f = \delta(E_a - E_b + \hbar\omega) \text{ with } E_b > E_a$$

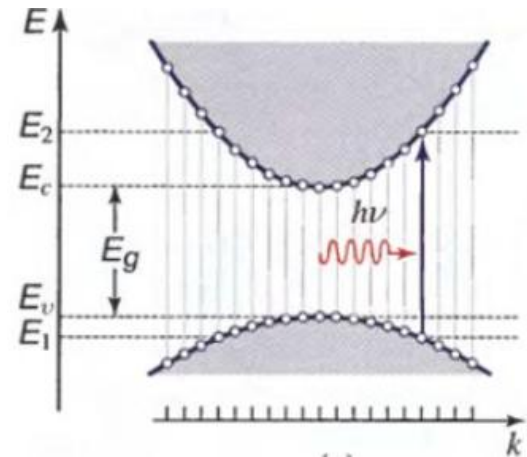
- Where ' M_{if} ' is the matrix element for the interaction
- ' ρ_f ' is density of final states (number of continuum states per unit volume)
- In a semiconductor, let us consider that the **state- a** in valence band is occupied and **state- b** in conduction band is empty.
- When a photon with energy greater than or equal to the bandgap of the semiconductor incidents, the electron moves from **state- a** in valence band to **state- b** in conduction band upon absorbing the photon (**Absorption**).

➤ According to **Fermi's Golden Rule**, the upward transition rate per unit volume is:

$$\text{Upward transition rate } W_{a \rightarrow b} = \frac{2\pi}{\hbar} |\langle b | H'(r)_{ab} | a \rangle|^2 \delta(E_a - E_b - \hbar\omega)$$

➤ By taking into consideration of

- All the initial states $\left(\sum_{K_a} \right)$ and final states $\left(\sum_{K_b} \right)$
- Probability of **state-*a*** being occupied (f_a)
- Probability of **state-*b*** being empty ($1-f_b$)
- The spin of electron (**prefactor '2'**)



Total upward transition rate per unit volume

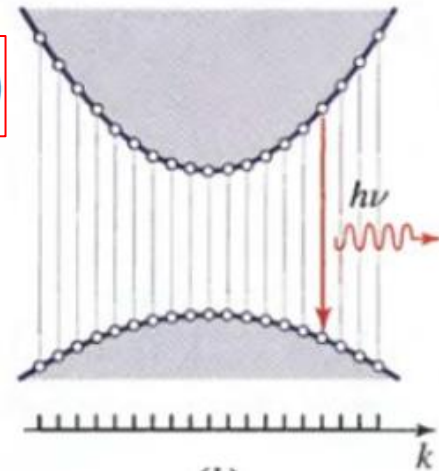
$$R_{a \rightarrow b} = \frac{2}{V} \sum_{K_a} \sum_{K_b} \frac{2\pi}{\hbar} |H'_{ab}|^2 \delta(E_b - E_a - \hbar\omega) f_a (1 - f_b)$$

- When the electron from **state-*b*** in conduction band comes back to **state-*a*** in valence band, releases a photon with energy less than or equal to the bandgap of the semiconductor(**Emission**).
- Following the same procedure as earlier:

$$\text{Downward transition rate } W_{b \rightarrow a} = \frac{2\pi}{\hbar} |\langle a | H'(r)_{ba} | b \rangle|^2 \delta(E_b - E_a + \hbar\omega)$$

Total downward transition rate per unit volume

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



Net Upward transition Rate:

The net upward transition rate per unit volume (R_n)

$$= R_{a \rightarrow b} - R_{b \rightarrow a}$$

$$\begin{aligned} \{\delta(E_a - E_b + \hbar\omega) &= \delta - (E_b - E_a - \hbar\omega) \\ &= \delta(E_b - E_a - \hbar\omega)\} \end{aligned}$$

$$|H'_{ba}| = |H'_{ab}|$$

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

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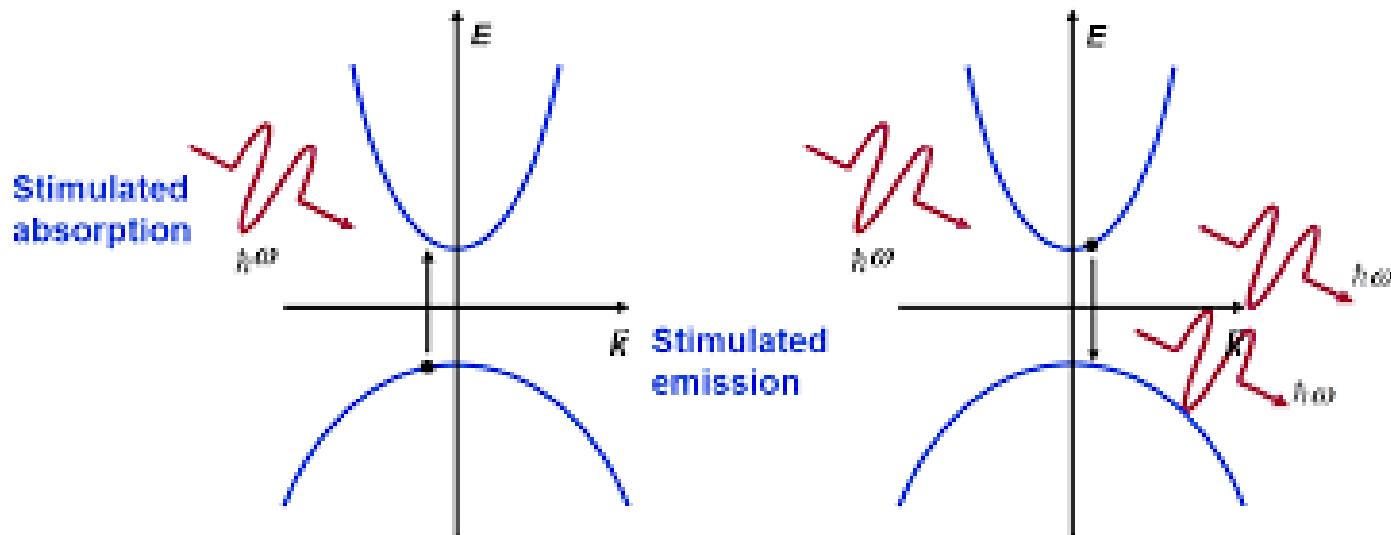
21PYB102J SEMICONDUCTOR PHYSICS AND COMPUTATIONAL METHODS

Session – 8 MODULE-III

Optical Gain and Optical Loss

Optical Gain:

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



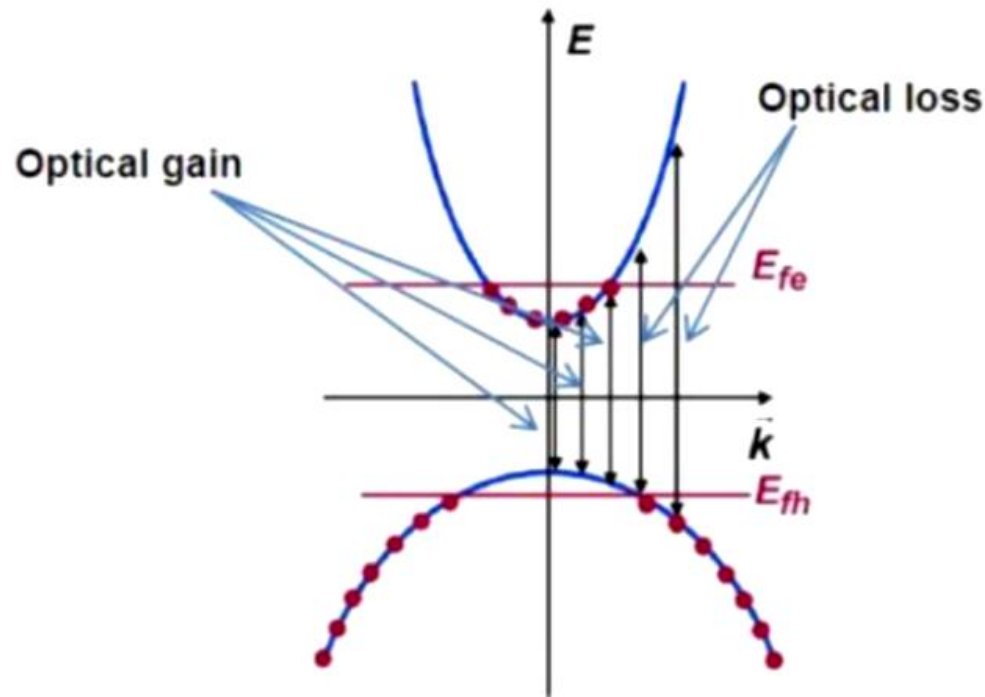
Optical Loss:

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



- Optical gain in a 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 a threshold value, such that the quasi-Fermi levels are separated by an energy greater than the band gap.
- If the number of downward transitions per seconds exceeds the number of upward transitions, 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.

- 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 condition for optical gain is net absorption process is greater than emission.



- From the above figure, given a value for the Fermi level splitting, optical frequencies for which $E_g < \hbar\omega < E_{fe} - E_{fh}$ experience optical gain.
- The condition $E_g < \hbar\omega < E_{fe} - E_{fh}$ is the condition for population inversion.
- From the above figure, given a value for the Fermi level splitting, optical frequencies for which $E_g > \hbar\omega, E_{fe} - E_{fh}$ experience optical loss.

Optical Gain and Loss from Fermi's Golden Rule:

- In a semiconductor crystal, consider an electron initially occupies a single state (b) and makes a transition to one of a large number of final states (a) 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.
- According to Fermi's Golden Rule:

$$\text{Upward transition rate } W_{a \rightarrow b} = \frac{2\pi}{\hbar} |H'_{ba}|^2 \rho_{red} f_a (1 - f_b)$$

$$\text{Downward transition rate } W_{b \rightarrow a} = \frac{2\pi}{\hbar} |H'_{ba}|^2 \rho_{red} f_b (1 - f_a)$$

ρ_{red} is reduced density of states

f_a and f_b are Fermi distribution functions

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 in unit time)
- ' z ' is the direction of the electromagnetic propagation

$$\frac{d\Phi}{dz} = W_{b \rightarrow a} - W_{a \rightarrow b}$$

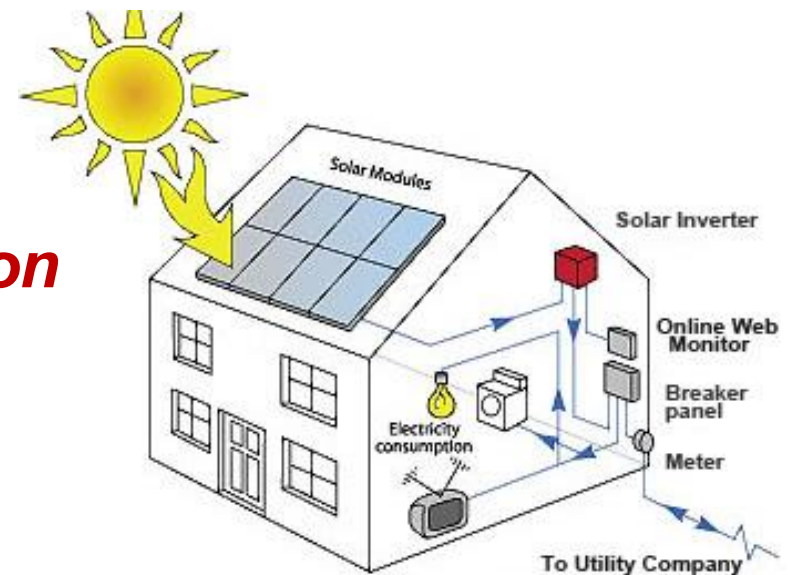
$$\text{Optical gain } (g) = \frac{1}{\Phi} \frac{2}{V} \sum_{K_a} \sum_{K_b} \frac{2\pi}{\hbar} |H'_{ba}|^2 \delta(E_a - E_b + \hbar\omega) (f_b - f_a)$$



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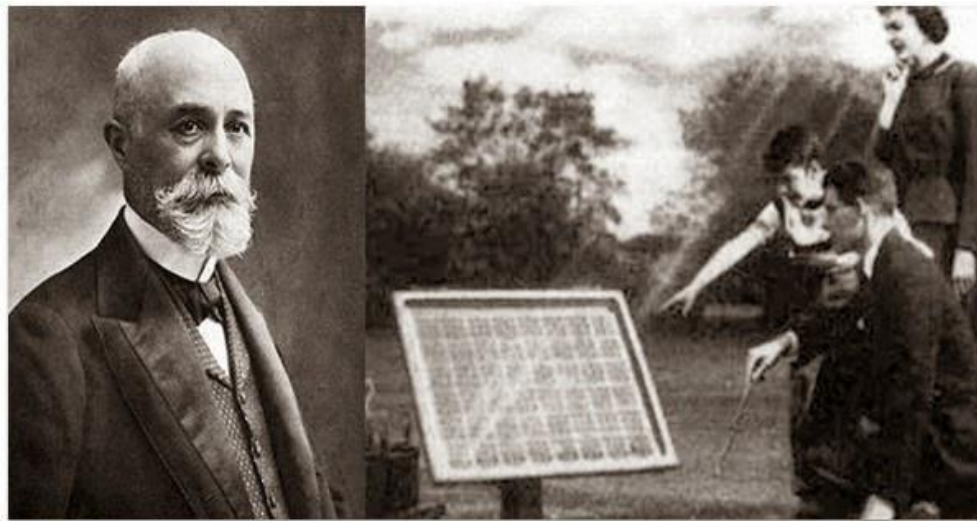
Photovoltaic Effect

Photovoltaic effect in PN Junction under illumination





Photovoltaic effect: It is a process that generates voltage or electric current in semiconductor device when it is exposed to light.



The photovoltaic effect was discovered in the year 1839 by French physicist, ***Edmond Becquerel***. It finds application in solar or photovoltaic cell to generate electricity.



History of Photovoltaic's

- *In 1839* – French physicist, *Edmond Becquerel* observed photovoltaic effect while experimenting with two silver-coated platinum electrodes immersed in a dilute acid and observed two electrodes altered their electric power under illumination.
- *In 1876* – *William G. Adams and Richard E. Day* who showed that electric power is directly produced under illumination.
- *In 1904* – *Albert Einstein* described the photoelectric effect on which photovoltaic technology is based.



- **1918** – A Polish scientist **Jan Czochralski** discovered a method for monocrystalline silicon production.
- **1941** – The first **photovoltaic monocrystalline** photovoltaic cell was constructed based on Czochralski method.
- **1951** – The first **germanium photovoltaic cells** was made in Bell's Laboratories with 4.5% efficiency.
- **1957** – **Hoffman Electronics** introduced photovoltaic cell with 8% efficiency and a year later, the efficiency of increased to 9% .



Introduction to solar radiation

Solar radiation is a radiant energy emitted by the sun as a result of its nuclear fusion reactions.

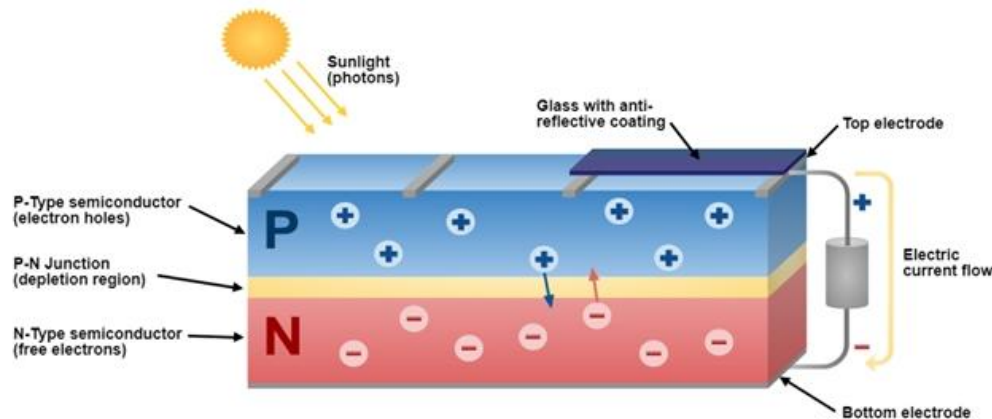
Over 99% of the energy flux from the sun is in the spectral region of $0.15 - 4\mu\text{m}$, with approximately 50% in the visible light region of $0.4 - 0.7\mu\text{m}$.

Sunlight is composed of photons and the photons contain different amounts of energy that correspond to the different wavelengths.



Photovoltaic in Semiconductor

The Solar or Photovoltaic cells are composed of two different types of semiconductor (a P-type and an N-type) that are joined together to create a PN Junction.





When photons strike a photovoltaic cell made by semiconductor PN junction, they may be reflected, absorbed or transmitted.

If photons is absorbed by the semiconductor then result is generation of electron-hole pair across PN Junction.

This electron-hole pair when separated from each other across the PN junction , results generation of voltage across the junction.

This voltage can drive a current in an external circuit called photocurrent

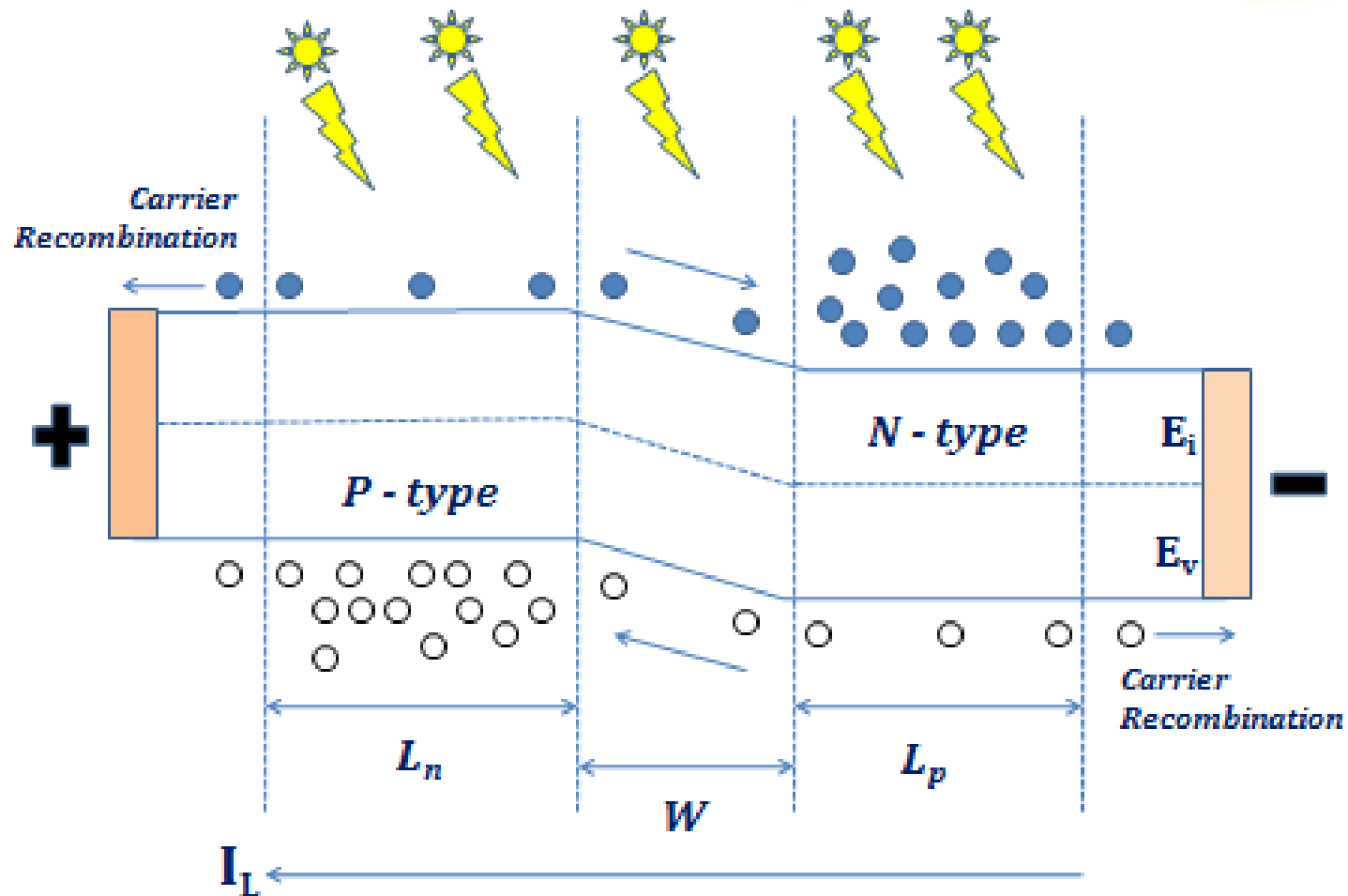


Photovoltaic in PN Junction under Illumination

When there is no light falling on the PN Junction, no electron-hole pair is generated. But when light is illuminated, it absorbs solar radiation and electron-hole pairs are generated.

Under the uniform illumination condition, generation of carrier will occur in the space-charge region as well as quasi-neutral region.

The carrier that are generated in the space charge region will be immediately swept away due to the electric field (electron towards N-region and holes towards P-region).



L_n and L_p - Diffusion length of electron and hole in Quasi neutral region, W - Width of depletion region or Space charge region, E_v - Energy of valence band and E_i - Fermi energy



Due to the electric field, chances of recombination of these electron pairs are quite less

The electron-hole pairs which are generated in the quasi neutral region will move around in a random manner.

In their random motion, some of the generated minority carriers will come near to the space charge region edge, where they will experience a force due to electric field and will be pulled at the other side

Only the minority charge carriers will cross the junction



Minority electrons from P-side will come to N-side leaving behind their positive charge called hole.

Similarly minority hole from N-side moves to P-side leaving behind their negative charge called electrons.

The drift of charge carriers creates a net increase in the positive charges at P-side and a net increase in negative charges at N-side.

This buildup of a positive and negative charge causes a potential difference to appear across the PN Junction under illumination. The potential difference created across light illuminated PN junction is called photo voltage.



The contribution to the photo voltage is coming only from the carriers that are generated within the semiconductor width ($L_n + W + L_p$)

Light generated Current

In a semiconductor PN Junction, four current components are present in equilibrium condition: drift current due to electron and hole, diffusion current due to electron and hole

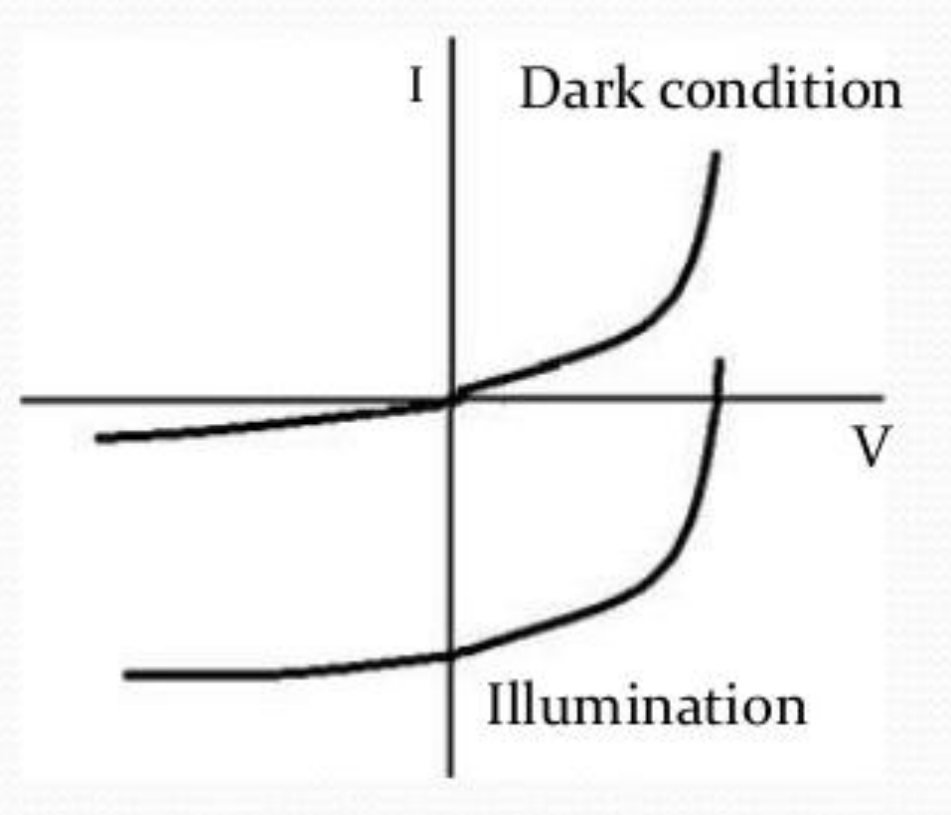
In equilibrium condition, net current is zero which requires the drift and diffusion currents of carriers to be equal and opposite.



When semiconductor PN Junction is illuminated, there is large drift current is observed due to minority electron and holes carrier.

Therefore in the I-V curve under dark, $I \propto V$ is observed as normally like PN diode.

But on illuminating the PN junction, large negative current caused by the light known as light generated current I_L is observed



Dark I-V curve and I-V curve under illuminated P-N Junction



The large negative current in illuminated PN junction is due to voltage which is generated due to light biases the PN Junction in a forward bias mode, the diffusion current flows opposite to the direction of light generated current

The light generated current is given by the following equation

$$I_{\text{total}} = I_0 (e^{qV/kT} - 1) - I_L$$

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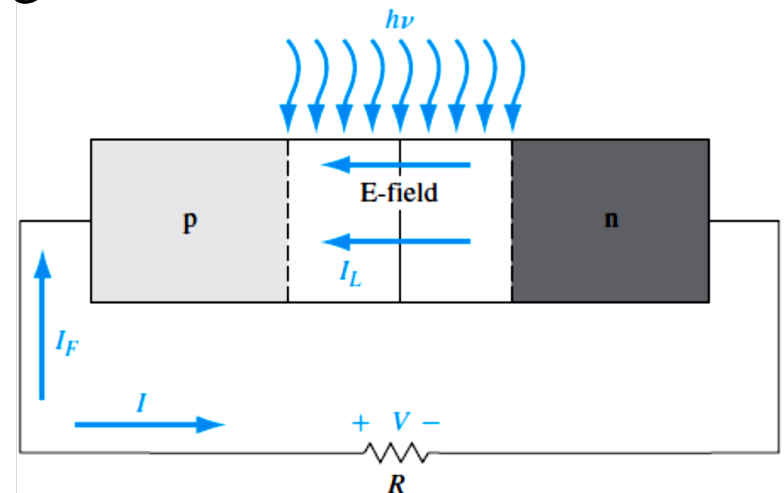
Solar Cell

A solar cell is a pn junction device with no voltage directly applied across the junction. The solar cell converts photon power into electrical power and delivers this power to a load.

The pn Junction Solar Cell

Consider the pn junction shown in Fig. 1, with a resistive load. Even with zero bias applied to the junction, an electric field exists in the space charge region as shown in the Fig. 1.

Figure 1 | A pn junction solar cell with resistive load.



Incident photon illumination can create electron-hole pairs in the space charge region that will be swept out producing the photocurrent I_L in the reverse-biased direction as shown in Fig. 1.

The photocurrent I_L produces a voltage drop across the resistive load which forward biases the pn junction. The forward-bias voltage produces a forward-bias current I_F as indicated in the Fig. 1.

The net pn junction current, in the reverse-biased direction, is

$$I = I_L - I_F = I_L - I_S \left[\exp\left(\frac{eV}{kT}\right) - 1 \right] \quad (1)$$

here the ideal diode equation has been used.

As the diode becomes forward biased, the magnitude of the electric field in the space charge region decreases, but does not go to zero or change direction. The photocurrent is always in the reverse-biased direction and the net solar cell current is also always in the reverse-biased direction.

There are *two limiting cases of interest*.

First limiting case is the *short-circuit condition* occurs when $\mathbf{R} = \mathbf{0}$ so that $V = 0$. The current in this case is referred to as the *short-circuit current*,

Or

$$I = I_{sc} = I_L \quad (2)$$

The *second limiting case* is the *open-circuit condition* and occurs when $R \rightarrow \infty$.

The net current is zero and the voltage produced is the *open-circuit voltage* V_{oc} . The photocurrent is just balanced by the forward-biased junction current, so we have

$$I = 0 = I_L - I_S \left[\exp\left(\frac{eV_{\infty}}{kT}\right) - 1 \right] \quad (3)$$

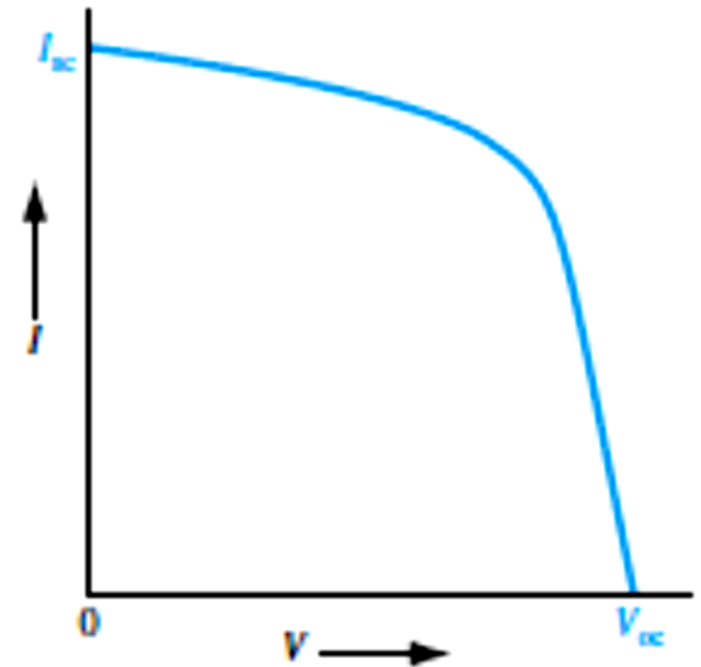
Then can find the open circuit voltage V_{oc} as

$$V_{OC} = V_t \ln\left(1 + \frac{I_L}{I_S}\right) \quad (4)$$

where $V_t = nkT/q$

A plot of the diode current I as a function of the diode voltage V from Eqn (4) is shown in Fig. 2. We may note the short-circuit current and open circuit voltage points on the figure.

Figure 2 | *I - V characteristics of a pn junction solar cell.*



The power delivered to the load is

$$P = V * I = I_L * V - I_S \left[\exp\left(\frac{eV}{kT}\right) - 1 \right] * V \quad (5)$$

We may find the current and voltage which will deliver the maximum power to the load by setting the derivative equal to zero, or $dP/dV = 0$.

Using Eqn. (5), we find

$$\frac{dP}{dV} = 0 = I_L - I_S \left[\exp\left(\frac{eV_m}{kT}\right) - 1 \right] - I_S V_m \left(\frac{eV}{kT} \right) \exp\left(\frac{eV_m}{kT}\right) \quad (6)$$

where V_m is the voltage that produces the maximum power.

We may rewrite Eqn. (6) in the form

$$\left(1 + \frac{V_m}{V_t} \right) \exp\left(\frac{eV_m}{kT}\right) = 1 + \frac{I_L}{I_S} \quad (7)$$

The value of V_m may be determined by trial and error. Figure 3 shows the maximum power rectangle where I_m is the current when $V = V_m$.

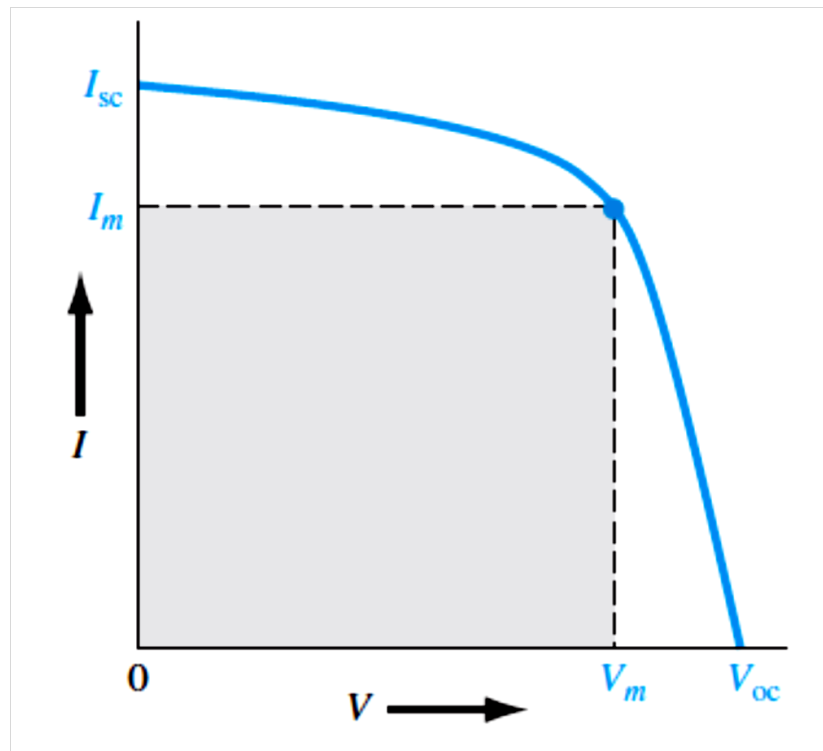


Figure 3 | Maximum power rectangle of the solar cell I - V characteristics.

Efficiency of a Solar Cell:

To determine the efficiency of the solar cell following parameters are to be described

➤ **Short-Circuit Current I_{sc}**

The short-circuit current is the current through the solar cell when the voltage across the solar cell is zero (i.e., when the solar cell is short circuited).

$$I_{sc} = -I_L \quad (8)$$

Here Short-Circuit Current is nothing but light generated current.

➤ Open-Circuit Voltage V_{oc}

The open-circuit voltage, V_{oc} , is the maximum voltage available from a solar cell, and this occurs at zero current. The open-circuit voltage corresponds to the amount of forward bias on the solar cell due to the bias of the solar cell junction with the light-generated current.

$$V_{oc} = \frac{nkT}{q} \ln\left(1 + \frac{I_L}{I_S}\right) \quad (9)$$

➤ Fill Factor FF

Fill Factor FF, is a measure of the realizable power from a solar cell. Typically, the fill factor is between 0.7 and 0.8. The FF is defined as the ratio of the maximum power from the solar cell to the product of V_{oc} and I_{sc} so that

$$FF = \frac{P_m}{I_{sc}V_{oc}} = \frac{I_m V_m}{I_{sc}V_{oc}} \quad (10)$$

➤ Conversion Efficiency η

The *conversion efficiency* η of a solar cell is defined as the ratio of output electrical power to incident optical power. For the maximum power output, we can write

$$\eta = \frac{P_m}{P_{in}} \times 100\% = \frac{I_m V_m}{P_{in}} \times 100\% = \frac{I_{sc} V_{oc} FF}{P_{in}} \times 100\% \quad (11)$$

The maximum possible current density and the maximum possible voltage in the solar cell are I_{sc} and V_{oc} , respectively.

The conventional pn junction solar cell has a single semiconductor bandgap energy. When the cell is exposed to the solar spectrum, a photon with energy less than E_g will have no effect on the electrical output power of the solar cell.

A photon with energy greater than E_g will contribute to the solar cell output power, but the fraction of photon energy that is greater than E_g will eventually only be dissipated as heat.

The maximum efficiency of a silicon pn junction solar cell is approximately 28 percent. Non ideal factors, such as series resistance and reflection from the semiconductor surface, will lower the conversion efficiency typically to the range of 10 to 15 percent.

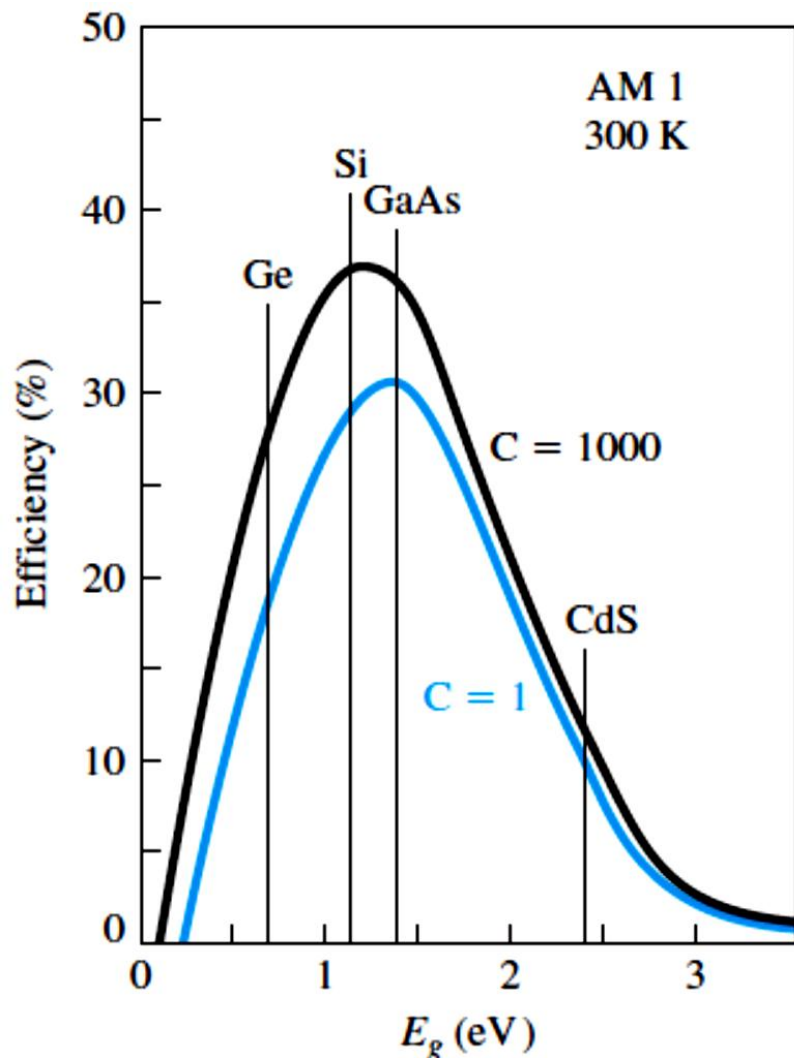


Figure 4 | Ideal solar cell efficiency at $T = 300$ K for $C = 1$ sun and for a $C = 1000$ sun concentrations as a function of bandgap energy.

A large optical lens can be used to concentrate sunlight onto a solar cell so that the light intensity can be increased up to several hundred times. The short-circuit current increases linearly with light concentration while the open-circuit voltage increases only slightly with concentration.

We can see that the conversion efficiency increases only slightly with optical concentration through Fig. 4. The primary advantage of using concentration techniques is to reduce the overall system cost since an optical lens is less expensive than an equivalent area of solar cells.

Loss in Solar Cell : Factors which affect Efficiency of the Solar Cell

1. Loss due to Low Energy Photons ($h\nu < E_g$)
2. Loss due to High Energy Photons ($h\nu > E_g$)
3. Voltage Loss
4. Fill Factor Loss
5. Loss due to Reflection
6. Loss due to less Absorption
7. Loss due to covering of Metal Contact
8. Recombination Loss