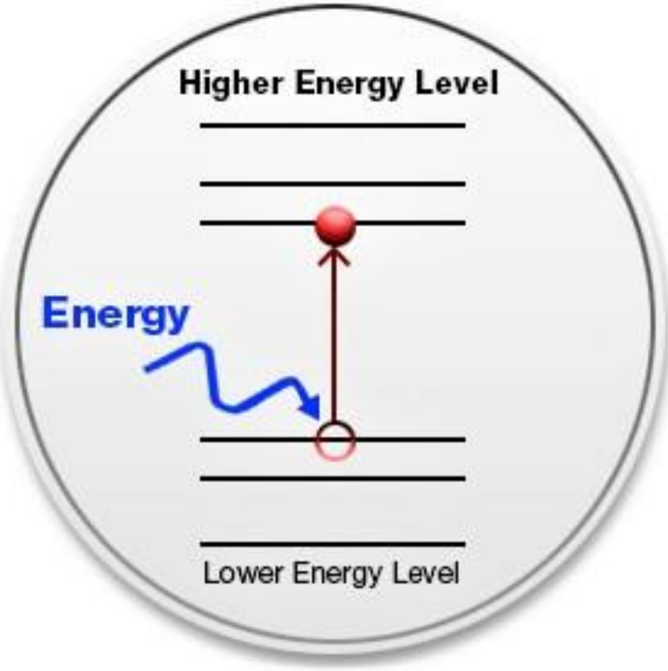
Chapter 2

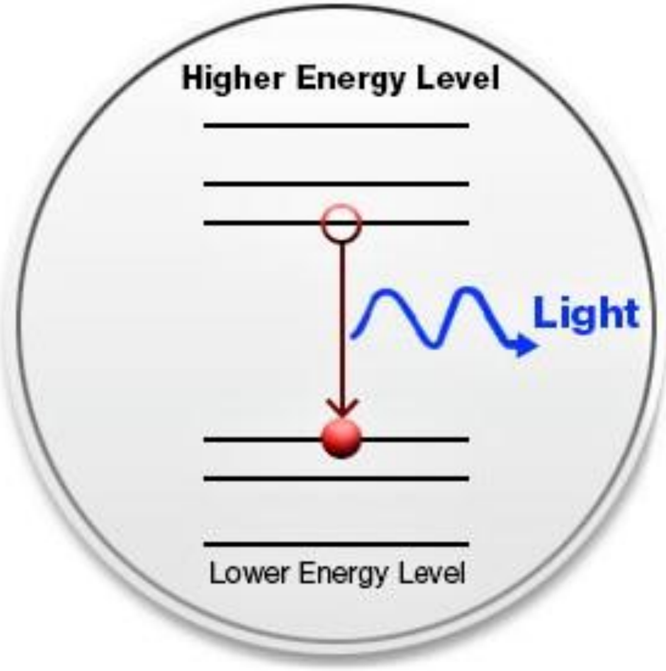
Optical and Electrical properties

- *Optical properties and material absorption*
- *Direct and indirect bandgap*
- *Absorption and absorption coefficient*
- *Generation rate and recombination*
- *Conductivity and carrier concentration*
- *Electron and Hole Mobilities*
- *Charge carriers path and velocity*

Optical properties

Optical property of a material is **defined** as **its** interaction with electro-magnetic radiation. ***Electromagnetic spectrum of radiation extents the wide range from γ-rays, through x-rays, ultraviolet, visible, infrared, and finally radio waves; the longest wavelengths in the spectrum.***



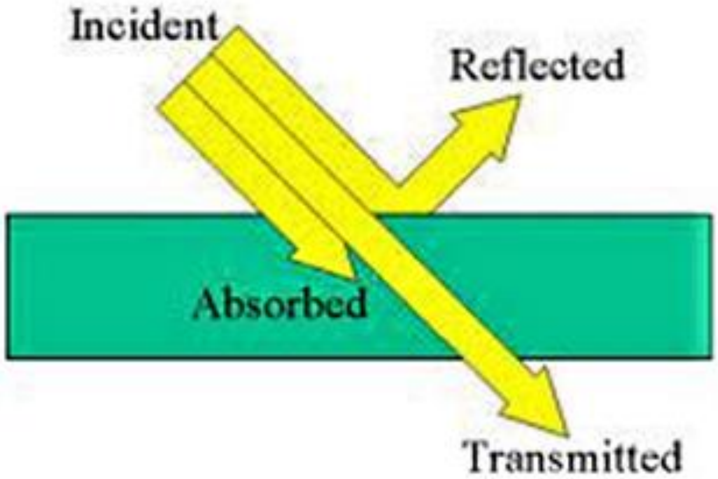


Optical properties

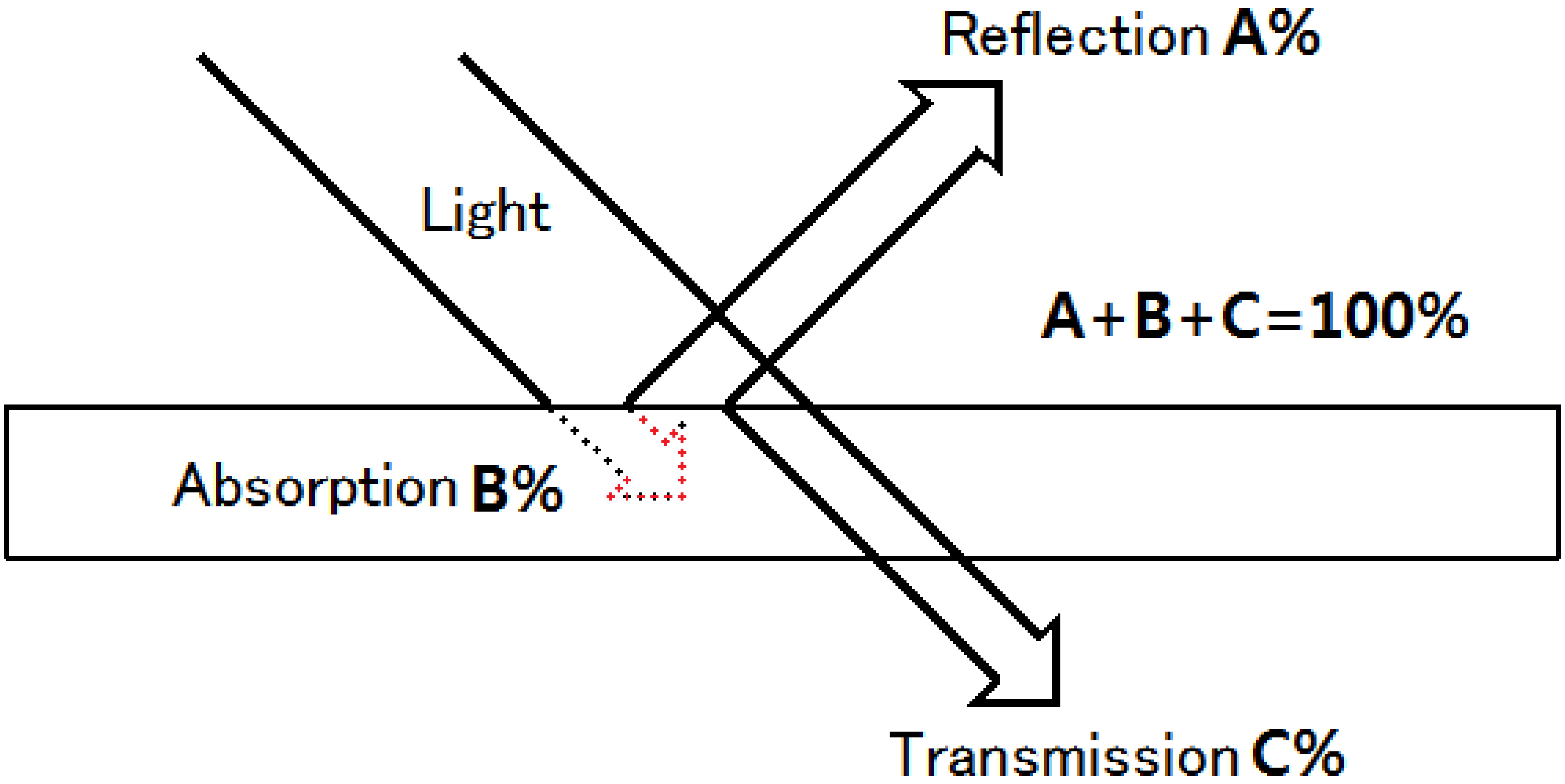
- To study a semiconductor optical properties, semiconductors absorb photons (light) and generate free charge carriers**.**
- **Absorption** in semiconductors occurs, when an electron absorbs a photon.
- **Absorption** therefore often leads to the **generation** of free charge carriers. Electron is excited into the conduction band, leaving a hole in the valence band.

- Photons, depending on their **energy** (corresponding wavelength), as well as on the **thickness and type of semiconductor material**, have various options: photons can be **transmitted** and passed right through the semiconductor (in which case the semiconductor is considered transparent), they can be **reflected** from the top surface, or they can be **absorbed**.

- **Transmitted** or **reflected** light is considered a loss, and therefore optical science is extremely important for minimizing the percentage of reflected light.



Light Reflection, Transmission, Absorption



Reflection **A%**

Light

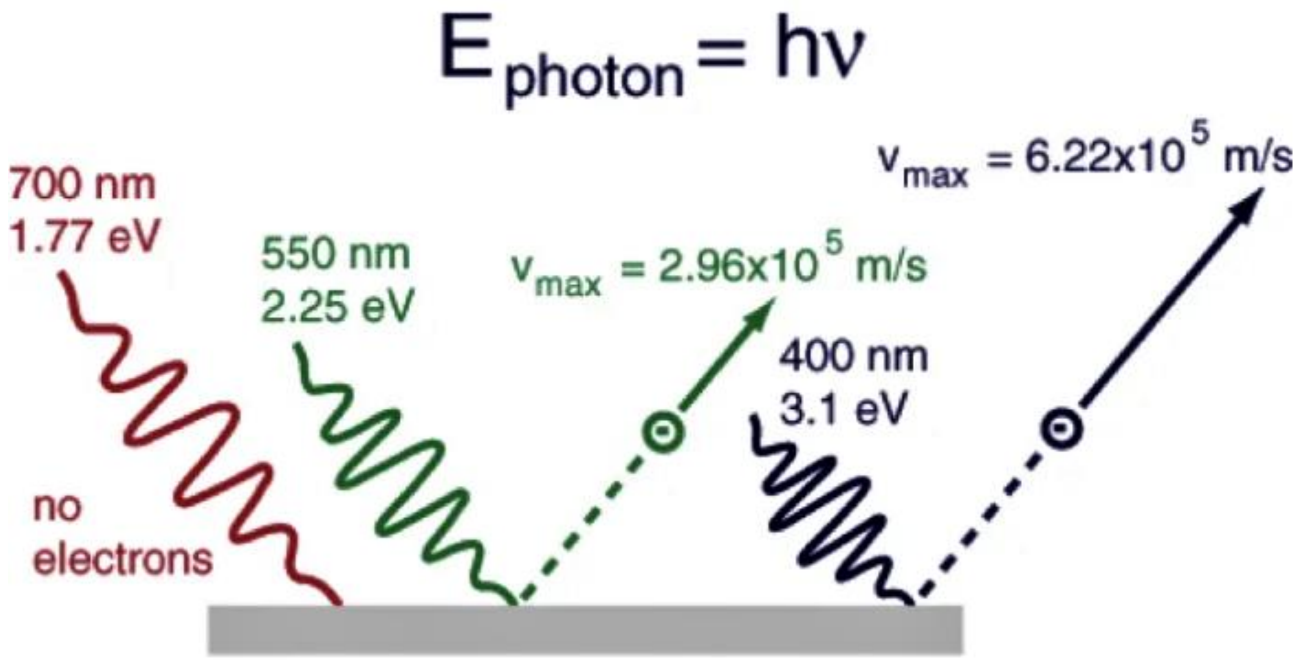
A+B+C=100%

Absorption **B%**

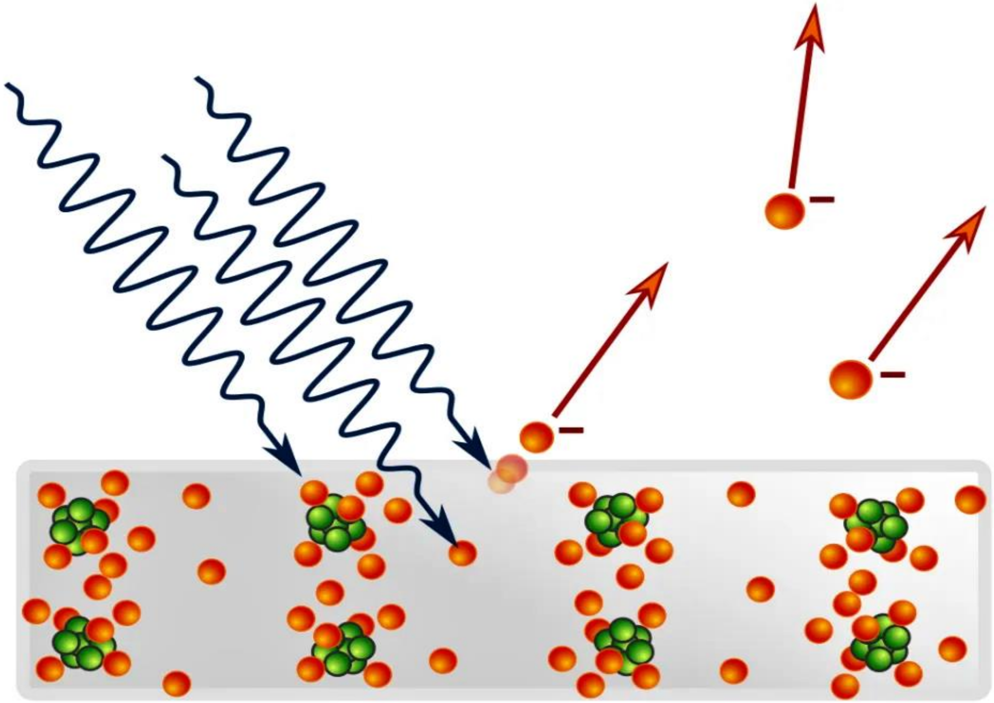
Transmission **C%**

Absorption and absorption coefficient

Absorption is the process in which incident photons lead to excite electrons from the valence band to the conduction band. The absorbed photons must have energy similar to that of the band gap of the semiconductor, $h\nu \geq E_g$. The process leads to an **optical** transition producing a hole in the valence band and an electron in the conduction band.



- ***Photons*** (**light**) incident on the surface of a semiconductor will be either **reflected** from the top surface, **absorbed** in the material or will be **transmitted** through the material. If the photon is absorbed, it has the possibility of exciting an electron from the valence band to the conduction band.



Note that, not all photons are absorbed:

- Photons, depending on their energy/corresponding wavelength, as well as on the thickness and type of semiconductor material;
- **options**: photons can be **transmitted** and passed right through the semiconductor (the semiconductor is considered **transparent**), they can be **reflected** from the top surface, or they can be **absorbed**.
- Transmitted or reflected light is considered a loss, and therefore optical science is extremely important for minimizing the percentage of reflected light

- For most cases of optical absorption, the energy absorbed is proportional to the thickness of the specimen.

$$I = I_0 e^{(-\alpha x)}$$

I**:** absorbed light intensity

I_0**:** initial intensity (incident)

α**:** absorption coefficient

x**:** the distance into the material at which the light intensity is being calculated

Absorption coefficient

- Absorption (**attenuation**) coefficient a measure of the rate of decrease in the intensity of light as it passes through a given substance

- It is the fraction of incident radiant energy absorbed per unit thickness of an absorber

- **The absorption coefficient determines how far into a material light of a particular wavelength can penetrate before it is absorbed**

- Material with a low absorption coefficient, light is only poorly absorbed, and if the material is thin enough, it will appear transparent to that wavelength.

- The absorption coefficient depends on the material and also on the wavelength of light which is being absorbed.

- Semiconductor materials have a ***sharp edge*** in their absorption coefficient. Light which has enough to excite an electron into the conduction band from the valence band is totally absorbed.

The SI unit of absorption coefficient is the reciprocal 1/cm (cm^{-1}).

Moreover, we can get the value of E_g by using the ***Tauc*** relation, which is given by this equation:

$$\alpha h\nu = A\,(h\nu - E_g)^n$$

where,

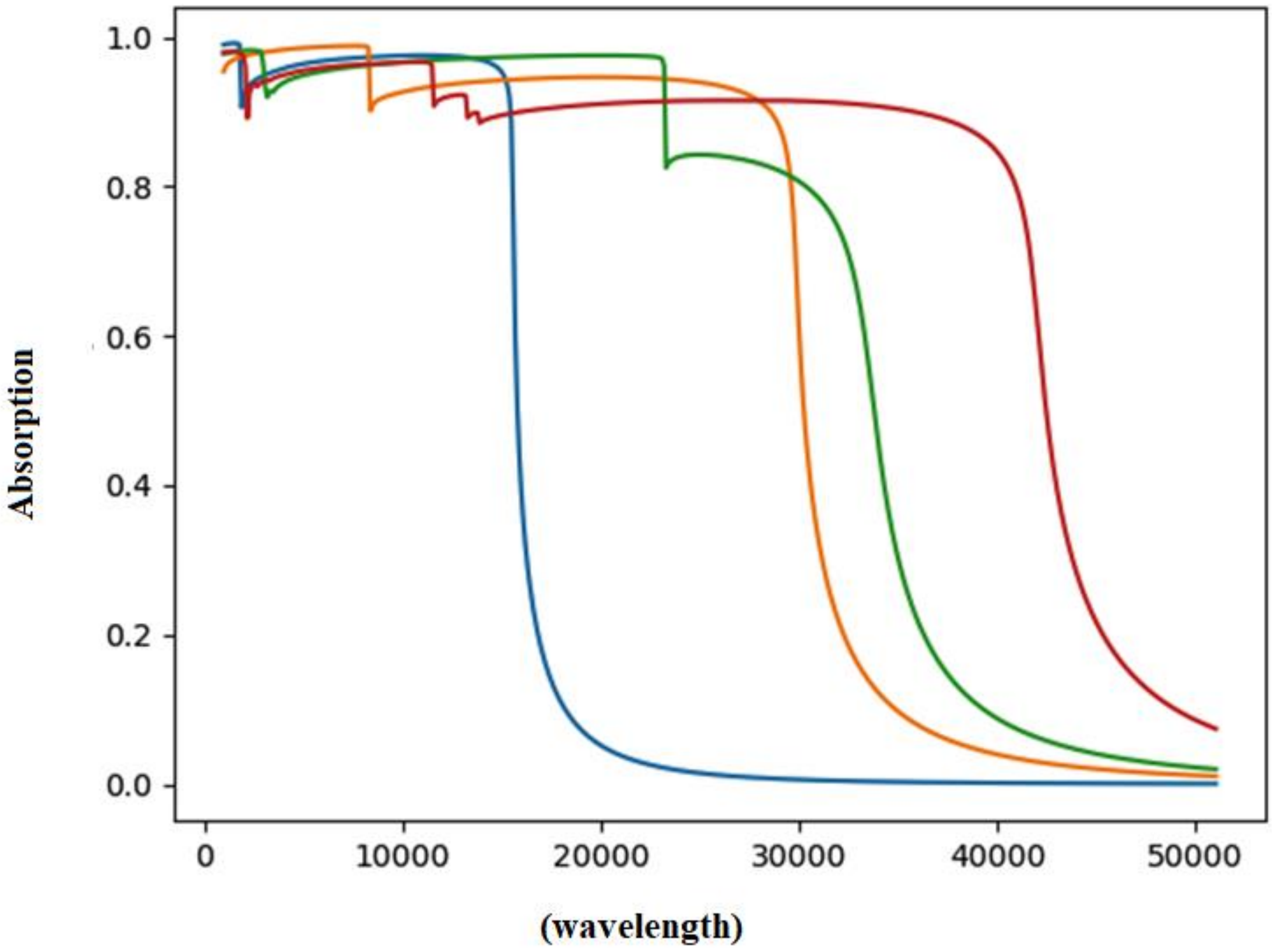
α = Absorption coefficient

$h\nu$ (eV) = 1240 incident wavelength (nm)

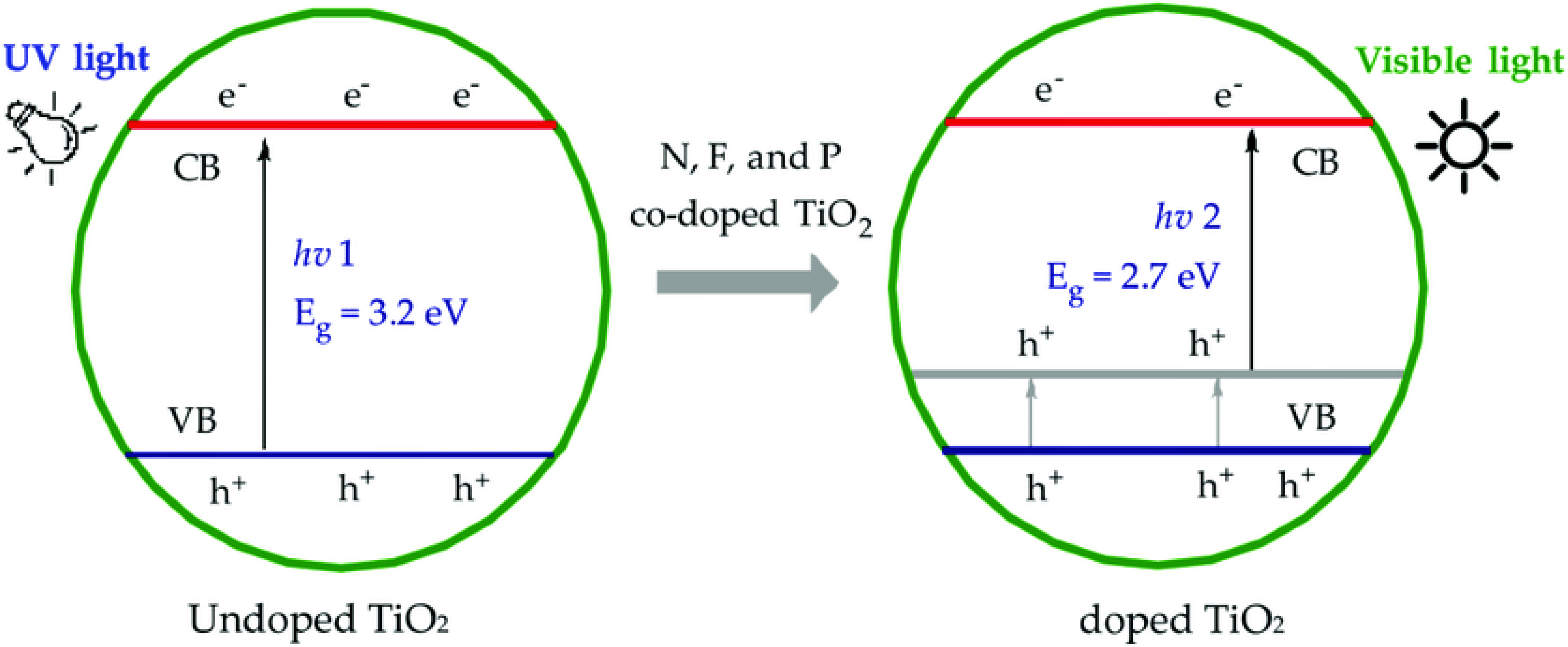
A = absorbance

n= 1/2 for direct allowed transition (direct energy gap)

n= 2 for indirect allowed transition (indirect energy gap)



Semiconductors have sharp edge of light absorption

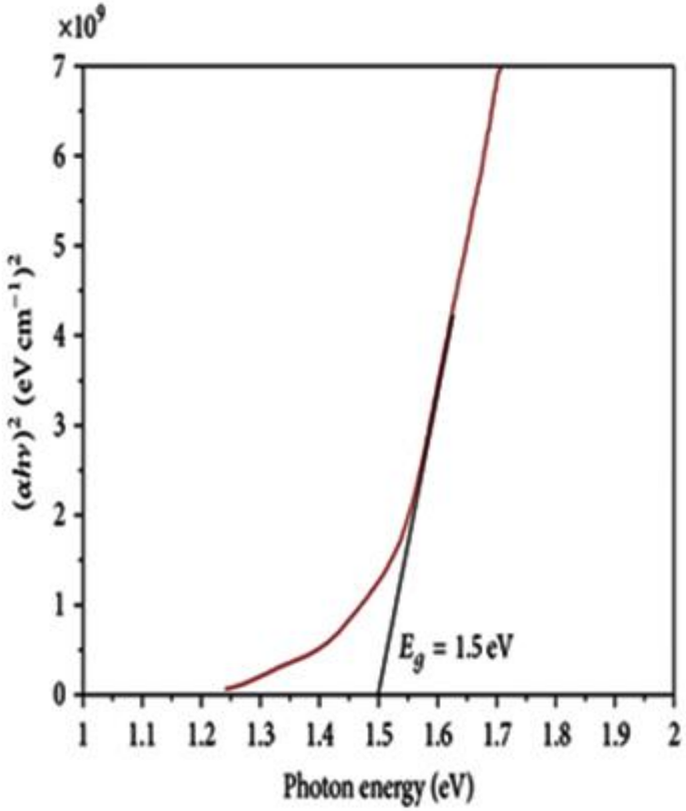

UV light
e-
e-
e-
CB
hv 1
Eg = 3.2 eV
VB
h+
h+
h+
Undoped TiO2
N, F, and P
co-doped TiO2
Visible light
e-
e-
CB
hv 2
Eg = 2.7 eV
h+
h+
VB
h+
h+
h+
doped TiO2

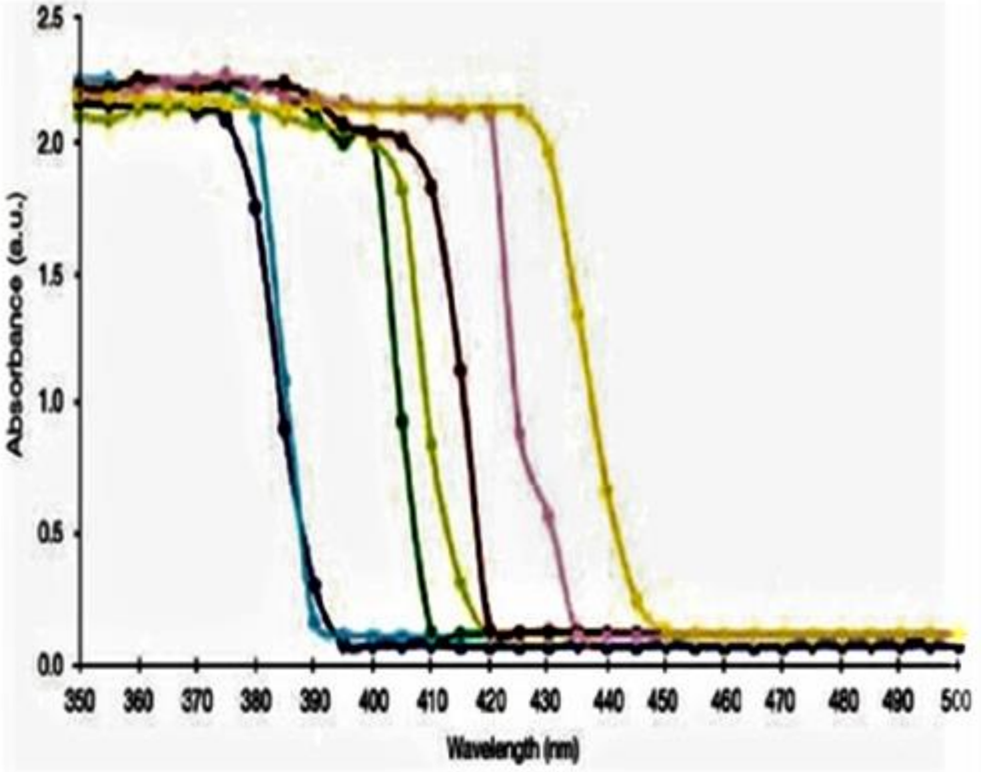
The **absorption coefficient** is related to the wavelength of light. It measures the rate of decrease in the intensity of light as it passes through a given substance; the fraction of incident energy absorbed per unit mass or thickness of an absorber.

- *how far into a material light of a particular wavelength can penetrate before it is absorbed.*
- *material with a low absorption coefficient, light is only poorly absorbed.*
- *The absorption coefficient depends on the material and also on the wavelength of light which is being absorbed*

It’s important to refer to that:

- ✓ Different semiconductor materials have different absorption coefficients.
- ✓ Materials with higher absorption coefficients more readily absorb photons, which excite electrons into the conduction band.
- ✓ Knowing the absorption coefficients of materials aids engineers in determining which material to use in their solar cell designs.
- ✓ Amount of light which is absorbed by a material depends on the absorption coefficient (α in cm^{-1}) and the thickness of the absorbing material


×10^9
7
6
5
4
3
2
1
0
(αhν)^2 (eV cm^−1)^2
1
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2
Photon energy (eV)
E_g = 1.5 eV


2.5
2.0
1.5
1.0
0.5
0.0
Absorbance (a.u.)
350
360
370
380
390
400
410
420
430
440
450
460
470
480
490
500
Wavelength (nm)

Absorption depth

- The absorption depth is a useful parameter which gives the distance into the material at which the light drops to about 36% of its original intensity

- The relationship between absorption coefficient and wavelength makes it so that different wavelengths penetrate different distances into a semiconductor before most of the light is absorbed.

- High energy light (short wavelength), such as blue light, has a large absorption coefficient, it is absorbed in a short distance (for silicon solar cells within a few microns) of the surface. ***Vise versa***

Q/ Determine the energy gap for an indirect band gap semiconductor knowing that, the absorption coefficient is 1.486 cm^{-1}, and the light absorbance was 0.12%.

Q/ Determine the attenuated light absorbed by a silicon slab thickness of 0.01 cm. Absorption coefficient of Si α = 1.5 cm^{-1}, incident intensity was about 175 $Watt/m^2$.

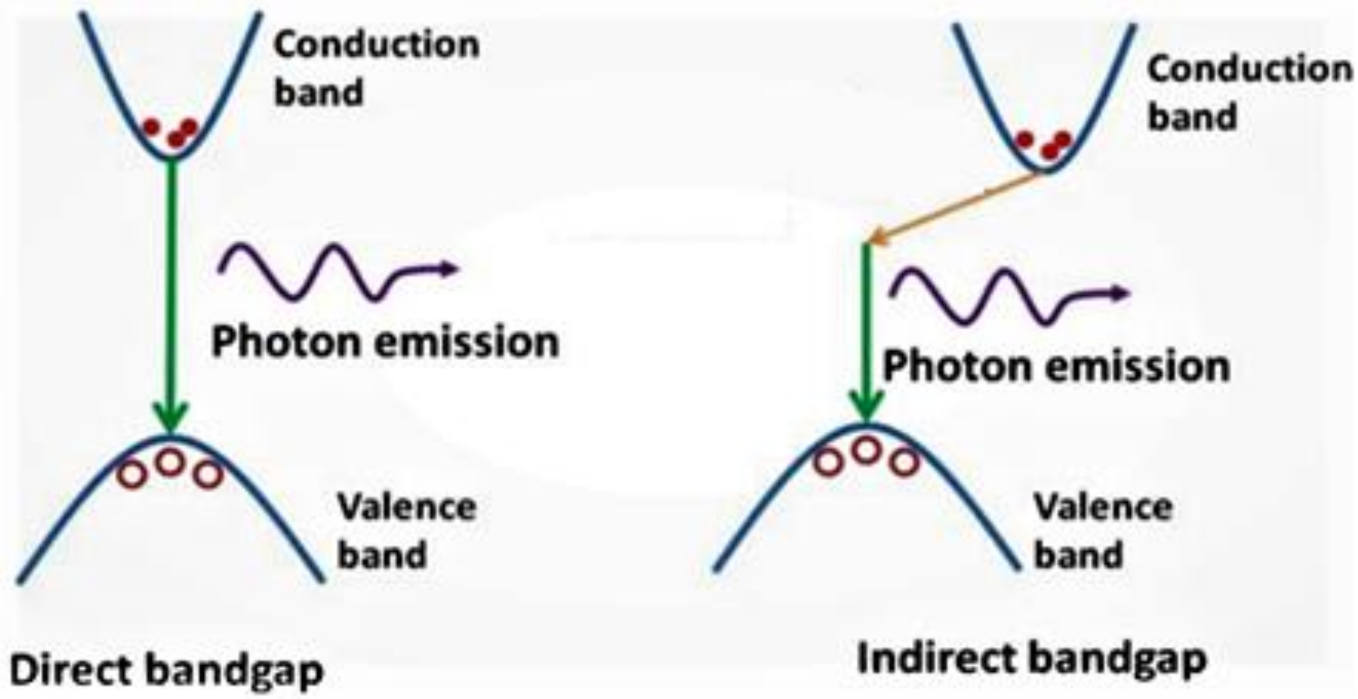
Q/ Determine the energy gap for a semiconductor exposed to 600 and 500 nm light wavelengths, knowing that no free electrons were generated.

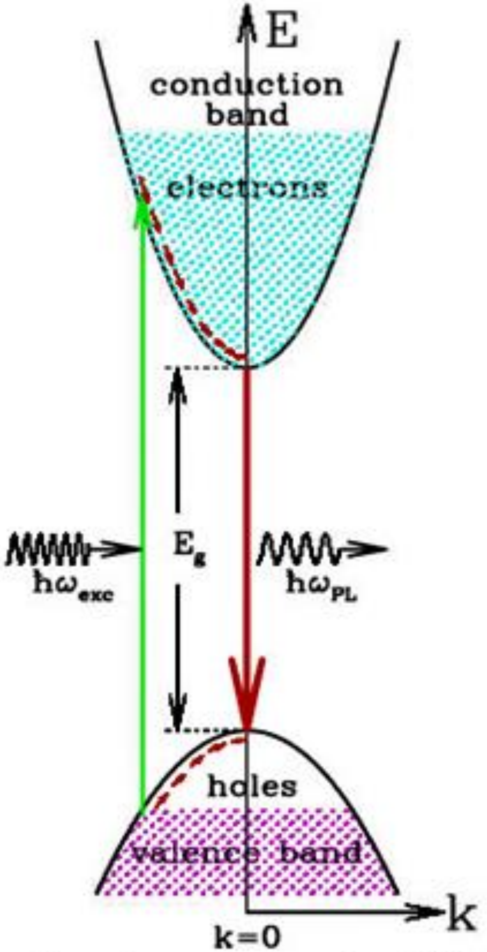
Q/ Calculate the light absorption depth for a silicon wafer thickness of 2mm, knowing that the incident light intensity was 0.5W/m^2 , Eg = 1.12 eV, A= 0.7.

Direct and indirect band gap

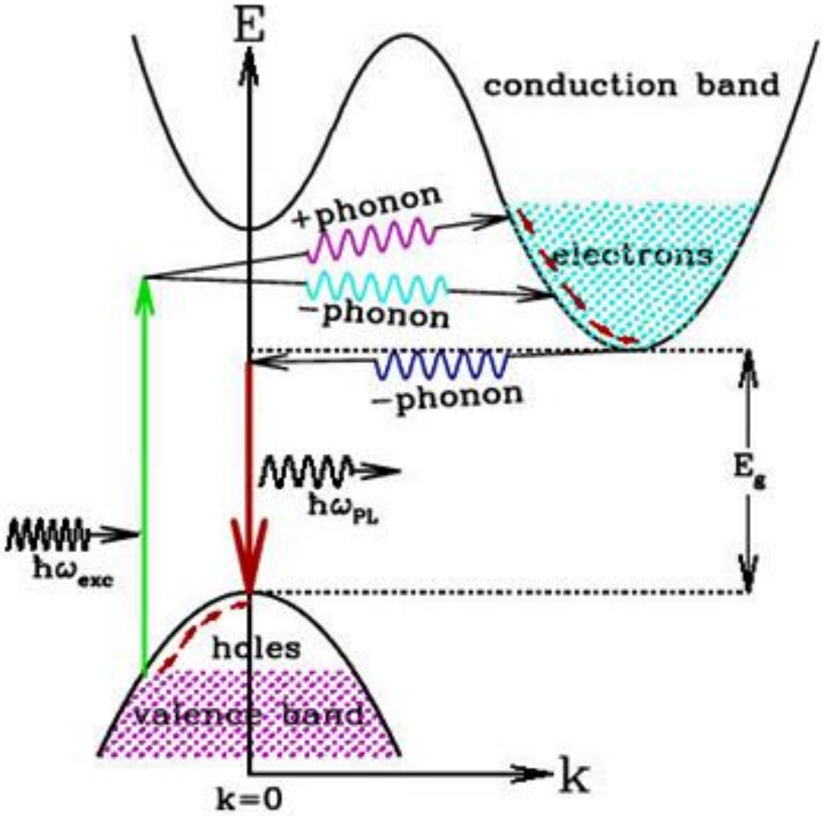
- In a direct band gap semiconductor, the top of the valence band and the bottom of the conduction band are both aligned.
- Electrons are excited and directly jump to the conduction band. Electrons are relaxed and back to the valance band when they loss their absorbed energy and this relaxation will be accompanied with light emission having an energy equal to the energy of the band gap energy.
- Electron transition known as band-to-band transition.

On the other hand, indirect bandgap the top of the valence band and the bottom of the conduction band are not aligned.



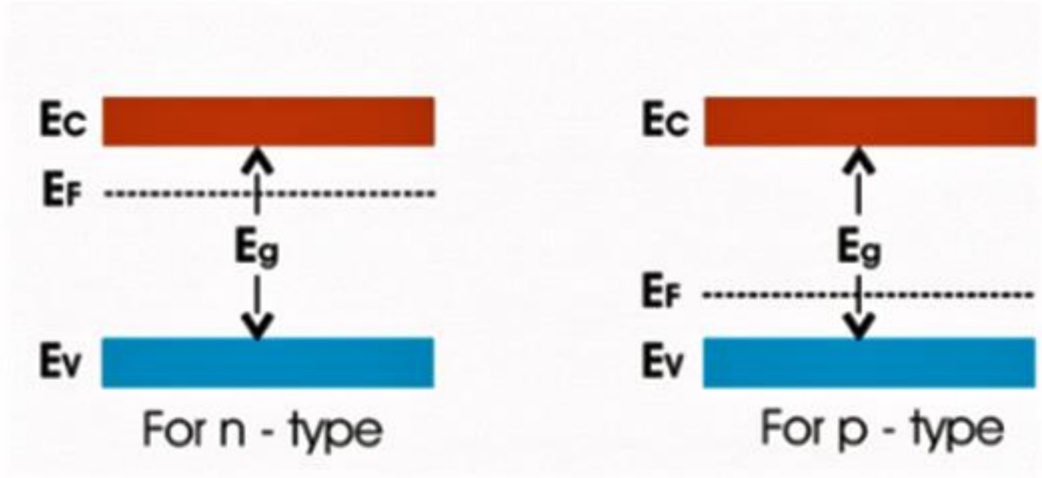


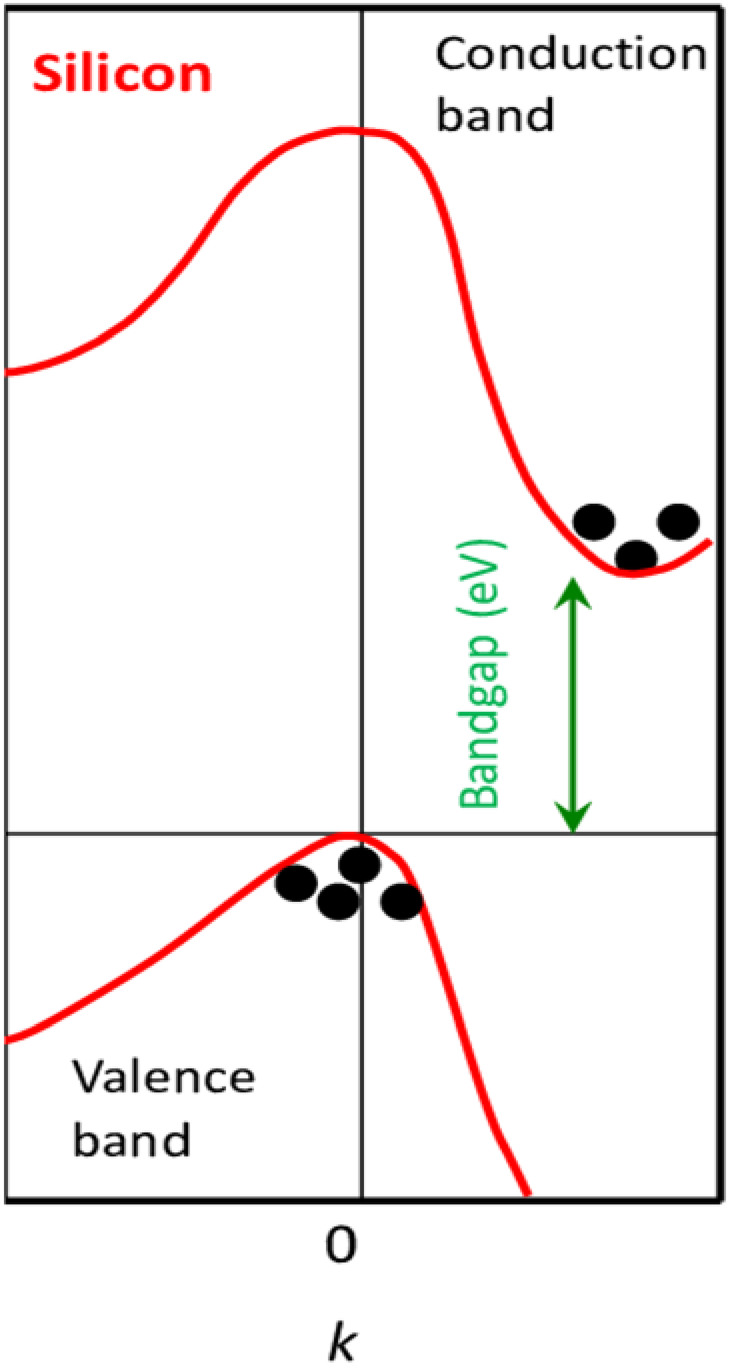
direct−gap materials



indirect−gap materials

What are Energy Bands of Silicon?





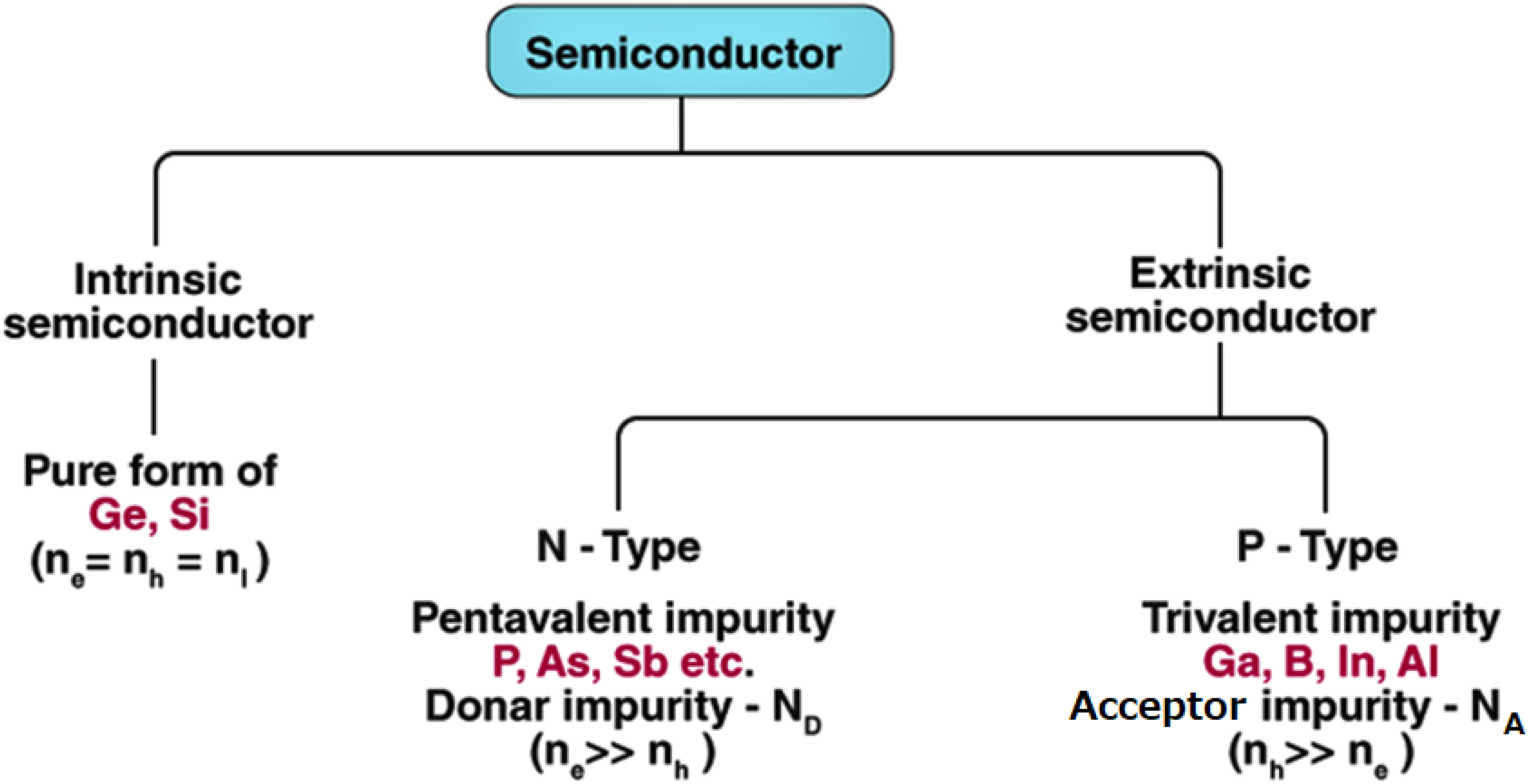
Generation rate

The generation rate gives the number of electrons generated at each point in the device due to the absorption of photons. Generation is an important parameter in solar cell operation.

Electrical properties of semiconductors

- Semiconductors in their natural state are poor conductors. There are several developed techniques that allow semiconducting materials to behave like conducting materials, by introducing impurities ("doping") into the structure.

- Impurities can either donate an electron to the conduction band, so called donors create n-doped materials, or accept an electron from the valence band, which are thereby called acceptors. Acceptors create p-doped materials with holes in the valence band left by the captured electron.



Semiconductor

Intrinsic semiconductor

Pure form of
Ge, Si
($n_e = n_h = n_i$)

Extrinsic semiconductor

N - Type

Pentavalent impurity
P, As, Sb etc.
Donar impurity - N_D
($n_e >> n_h$)

P - Type

Trivalent impurity
Ga, B, In, Al
Acceptor impurity - N_A
($n_h >> n_e$)

- * n-type (Donor)
- * 5 valence electrons

- * p-type (Acceptor)
- * 3 valence electrons

Intrinsic Fermi level position, E_{Fi}

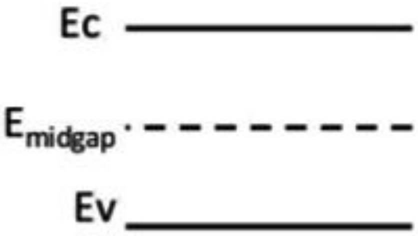
If E_F closer to Ec, n>p
If E_F closer to Ev, n<p

Intrinsic; n=p ⇓

E_F is located near the center of the forbidden bandgap

$$N_C \exp\left[\frac{-(E_C - E_{Fi})}{kT}\right] = N_v \exp\left[\frac{-(E_{Fi} - E_v)}{kT}\right]$$

$$E_{Fi} = E_{midgap} + \frac{3}{4} kT \ln\left(\frac{m_p^*}{m_n^*}\right)$$



$M_p = m_n$ ➡ $E_{Fi} = E_{midgap}$

$M_p \neq m_n$ ➡ E_{Fi} shifts slightly from E_{midgap}

n-type semiconductor

- In n-type semiconductors pentavalent impurity (e.g. arsenic As in Si, or Phosphorus P) is added to an intrinsic semiconductor. These impurities are called donors.

- The addition of pentavalent impurity creates large number of free electrons in the conduction band. At room temperature, the number of electrons is greater than the number of holes. Electrons are said to be the majority carriers whereas holes are the minority carriers.

- The semiconductor will have a higher electron density. Therefore, in the n-type semiconductor when the donor density is increased, the ***Fermi level*** moves closer to the conduction band.

- The Fermi level for n-type semiconductor is given as:

$$E_C - E_F = kT\ln\left(\frac{N_C}{n_o}\right)$$

Compensated semiconductor, $n_o = N_d - N_a$

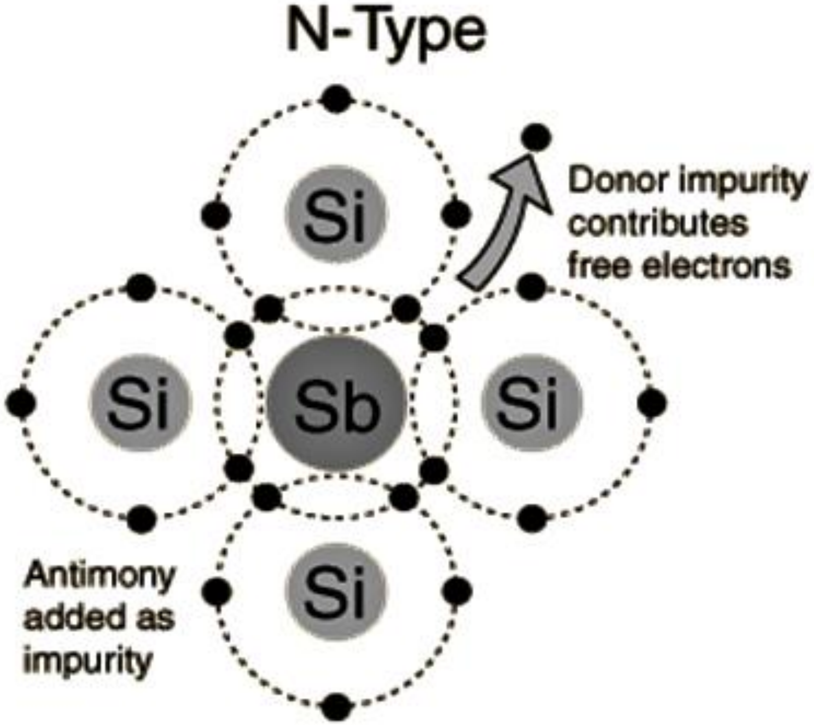
$$E_C - E_F = kT\ln\left(\frac{N_C}{N_d - N_a}\right)$$

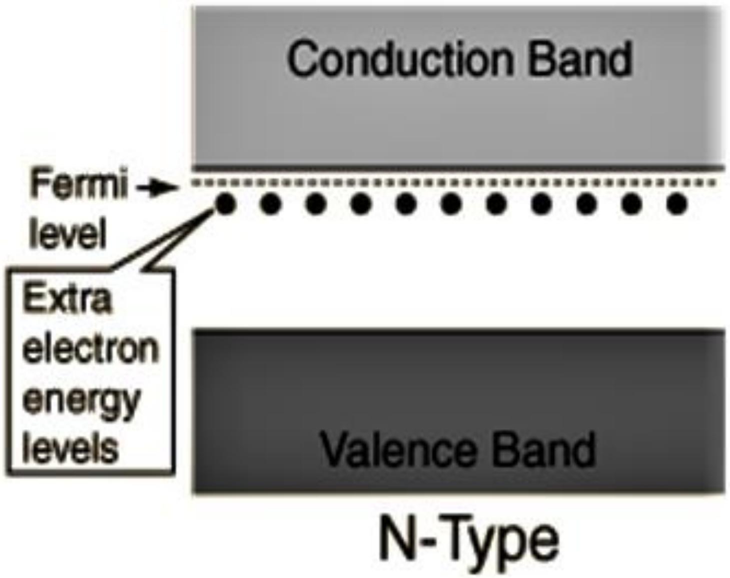
$$E_F - E_{Fi} = kT\ln\left(\frac{n_o}{n_i}\right)$$

Where,

E_C the energy of the conduction band
E_F is the Fermi level
K is the Boltzmann constant
T is the absolute temperature
N_C the effective density of electrons
N_d is the concentration of donor atoms
N_a is the concentration of acceptor atoms
$n_\circ$ is the concentration of electrons

The important points regarding n-type semiconductors are summarized graphically in the figures below:





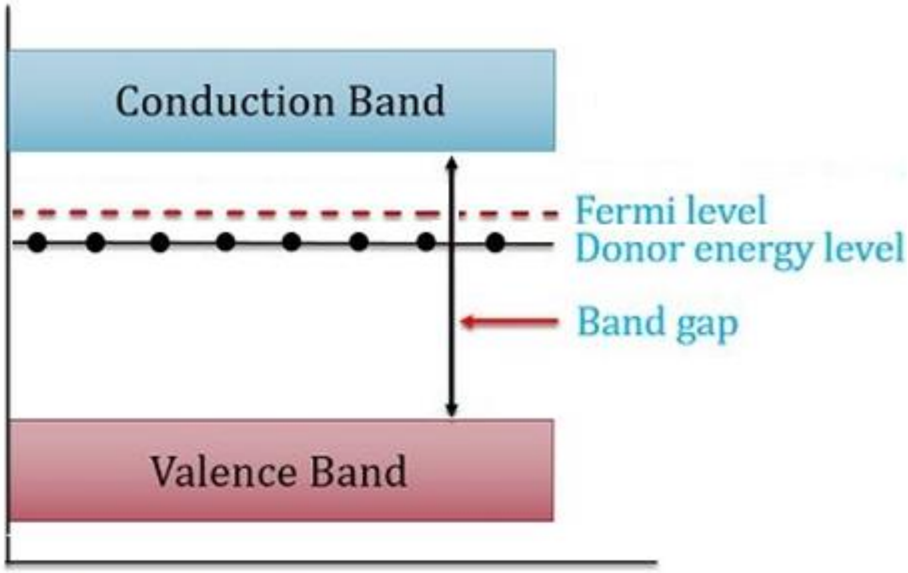
Donor Level

- **Donor** is a dopant atom that, when added to a semiconductor, can form an **n-type** semiconductor.

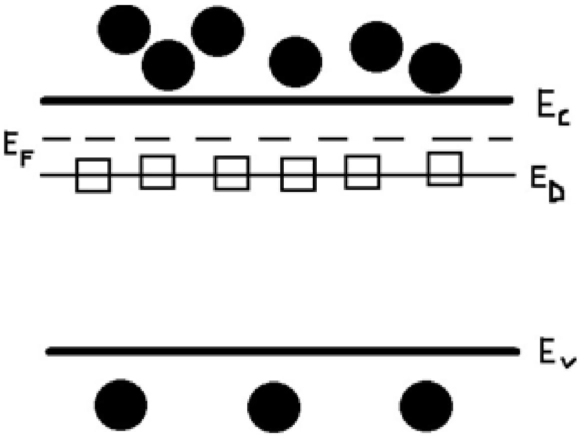
- From the energy gap viewpoint, such impurities “create” energy levels in the band gap close to conduction band so that electrons can be easily excited from these levels into the conduction band.

- Therefore, the conductivity of an n-type semiconductor increases at even below the room temperature. The electrons are said to be the “**majority carriers**” for current flow in an n-type semiconductor.

- This shifts the ***Fermi level*** to a point about halfway between the donor levels and the conduction band.



Energy level diagram of N type semiconductor

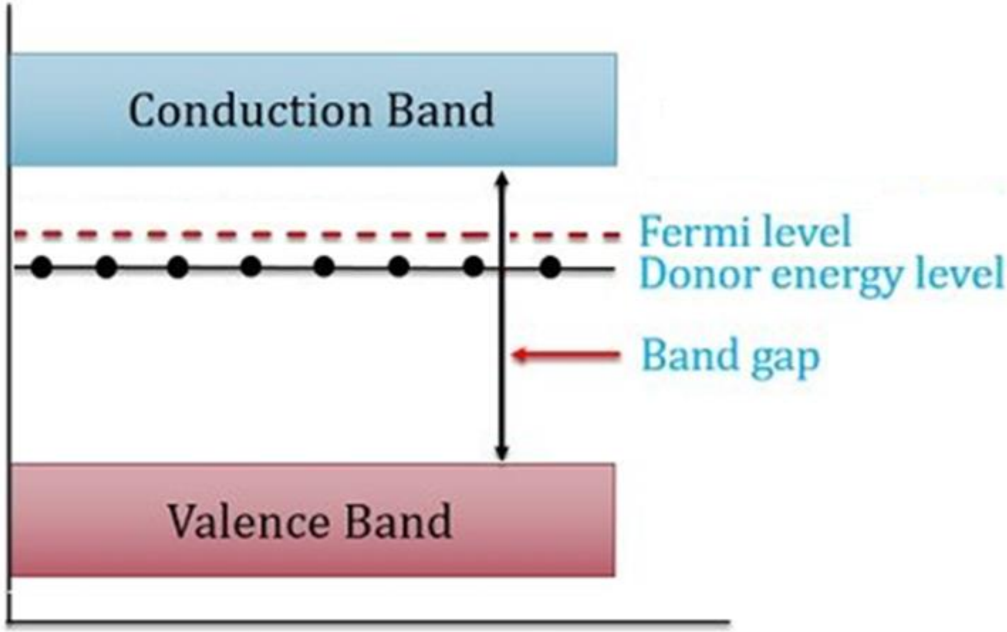


$$n_d = \frac{N_d}{1+\frac{1}{2}\exp\left(\frac{E_d - E_F}{kT}\right)} = N_d - N_d^+$$

Density of electron occupying the donor level

Concentration of donors

Concentration of ionized donors



Energy level diagram of N type semiconductor

AS an important calculation, is to find the concentration of electrons in the conduction band. At room temperature, this concentration is simply n_o

$$n_o = N_C \exp\left[\frac{-(E_C - E_F)}{kT}\right]$$ concentration of electron

N_c: the effective density of electrons

E_c: the energy of the conduction band

E_F: the energy of fermi level

K is the Boltzmann constant

T is the absolute temperature

Intrinsic or pure semiconductors:

1. Very chemically pure.

2. Possesses a very low conductivity level having very few numbers of charge carriers.

3. Electrons and holes are existed in equal quantities.

4. Fermi level lies in the middle of the energy band gap.

p-type semiconductor

- In p-type semiconductors trivalent impurity (e.g. boron B or Al in Si) is added to an intrinsic semiconductor. These impurities are called acceptors.

- The addition of trivalent impurity creates large number of holes in the valance band. At room temperature, the number of holes is greater than the number of electrons. Holes are said to be the majority carriers whereas electrons are the minority carriers.

- The semiconductor will have a higher hole density. Therefore, in the p-type semiconductor when the acceptor density is increased, the ***Fermi level*** moves closer to the valance band.

- The Fermi level for p-type semiconductor is given as:

$$E_F - E_C = kT \ln\left(\frac{N_v}{p_o}\right)$$

Compensated semiconductor, $p_o = N_a - N_d$

$$E_F - E_v = kT \ln\left(\frac{N_v}{N_a - N_d}\right)$$

$$E_{Fi} - E_F = kT \ln\left(\frac{p_o}{n_i}\right)$$

Where,

E_C the energy of the conduction band

E_F is the Fermi level

K is the Boltzmann constant

T is the absolute temperature

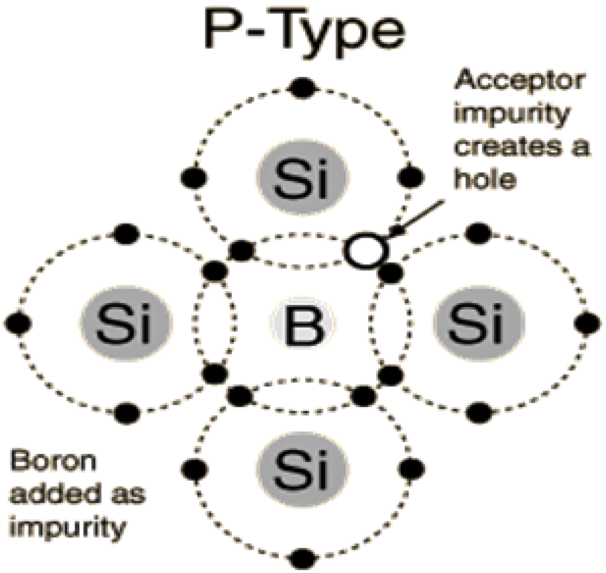
N_V the effective density of holes

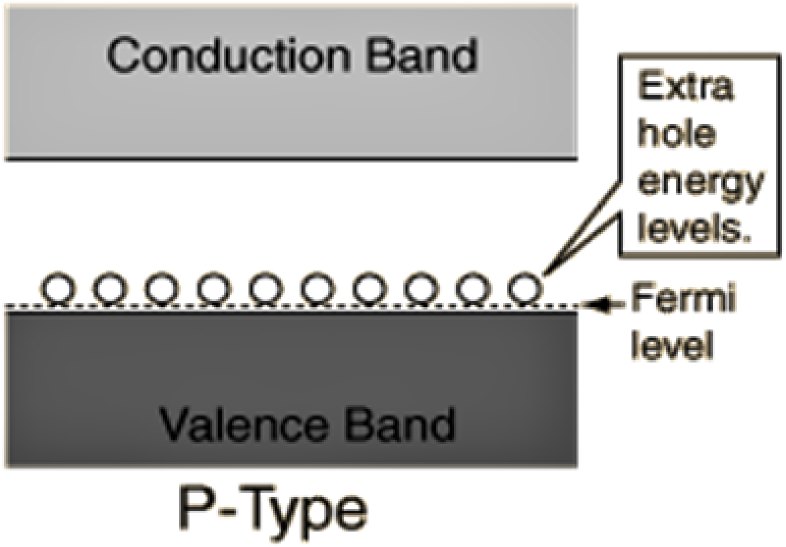
N_d is the concentration of donor atoms

N_a is the concentration of acceptor atoms

$p_\circ$ is the concentration of holes

The important points regarding p-type semiconductors are summarized graphically in the figures below:





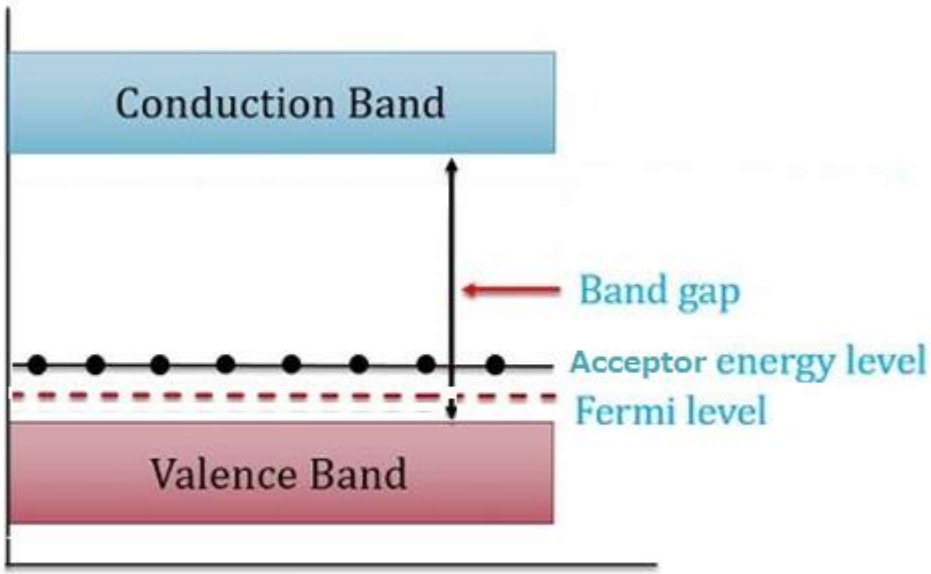
Acceptor Level

- **Acceptor** is a dopant atom that, when added to a semiconductor, can form a **p-type** semiconductor.

- From the energy gap viewpoint, such impurities "create" energy levels in the band gap close to valance band known as acceptor level.

- Therefore, the conductivity of a p-type semiconductor increases at even below the room temperature. Holes are said to be the "**majority carriers**" for current flow in an p-type semiconductor.

- This shifts the ***Fermi level*** to a point about halfway between the acceptor levels and the valance band (see the figure).



Energy level diagram of p type semiconductor

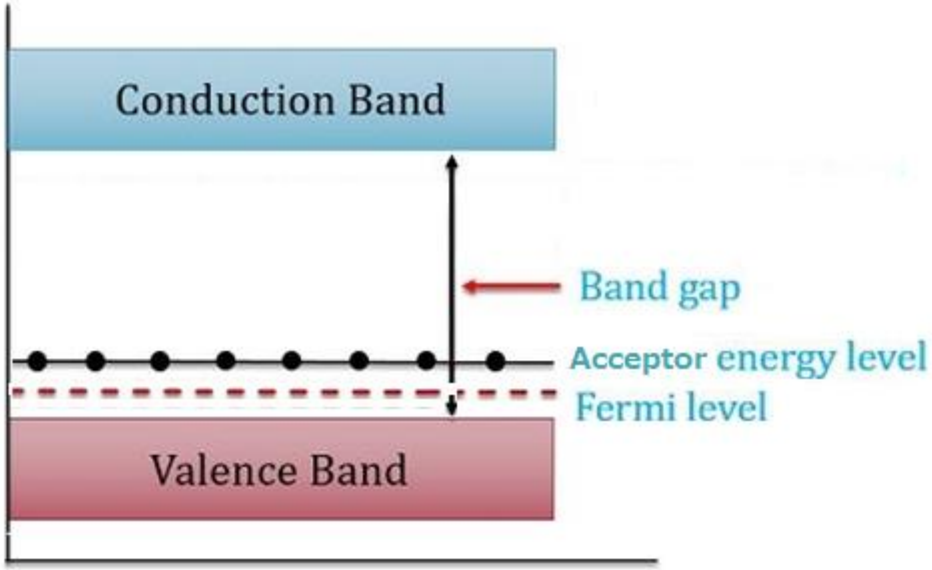
$$p_a = \frac{N_a}{1+\frac{1}{g}\exp\left(\frac{E_F - E_a}{kT}\right)} = N_a - N_a^-$$

Concentration of holes in the acceptor states

Concentration of acceptors

Concentration of ionized acceptor

g; degeneracy factor (Si; 4)



Energy level diagram of p type semiconductor

AS an important calculation, is to find the concentration of holes in the valance band. At room temperature, this concentration is simply P_o

$$p_o = N_v \exp\left[\frac{-(E_F - E_v)}{kT}\right]$$

concentration of hole

N_V: the effective density of holes

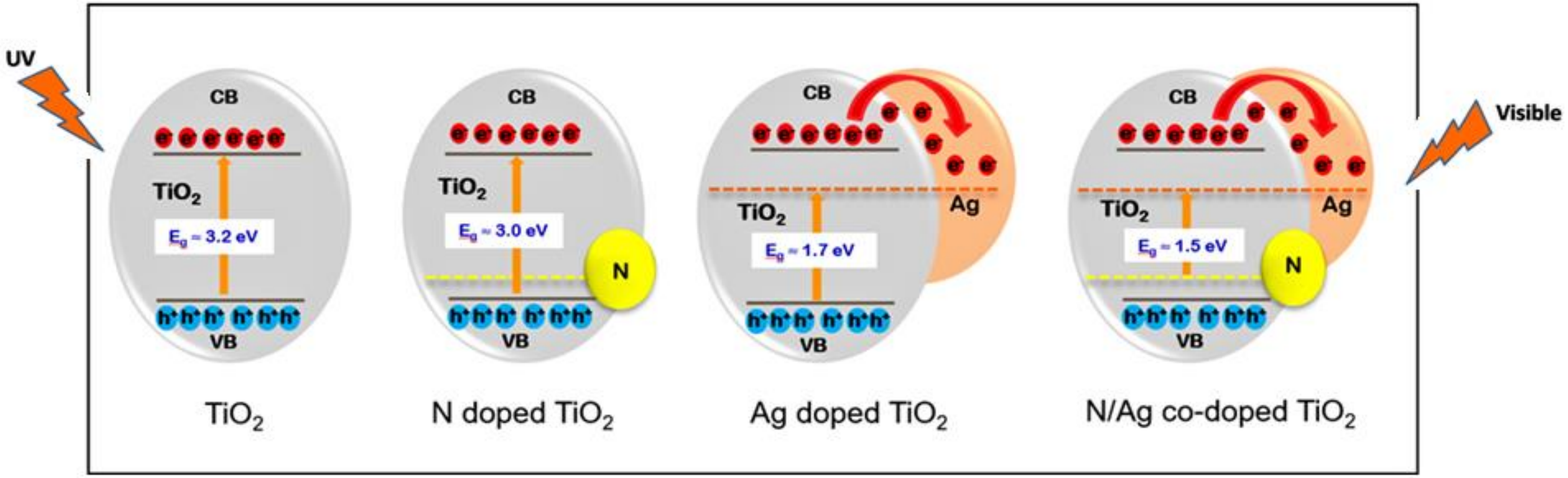
E_V: the energy of the valance band

E_F: the energy of fermi level

K is the Boltzmann constant

T is the absolute temperature

- It is important to refer that, doping of a semiconductor improves the light response range of the material. By determining doping parameters such as the band gap of dopants and the doping concentration, the band gap of the doped semiconductor can be tuned (adjusted) to the desired energy gap and absorbed light wavelength.



TiO_2 N doped TiO_2 Ag doped TiO_2 N/Ag co-doped TiO_2

Defects in semiconductors

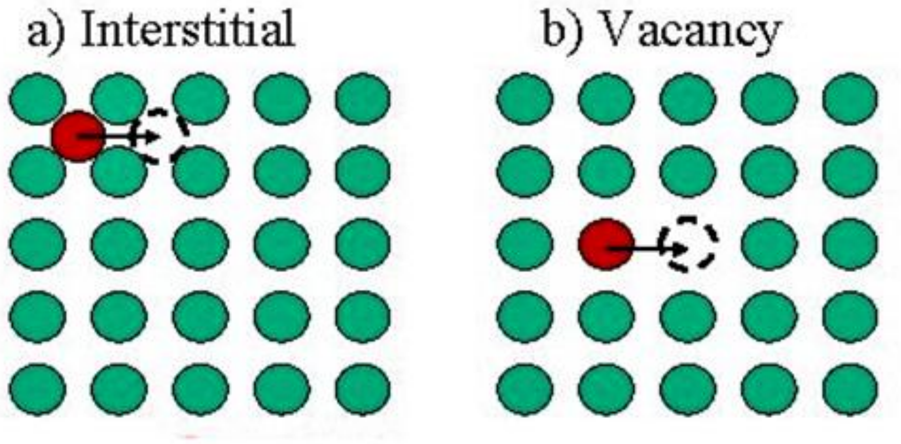
- Like anything else in this world, semiconductors possess imperfections, or what often refer to as ***'defects'***. The presence of most of these defects is undesirable. Defects in semiconductors fall into two categories:

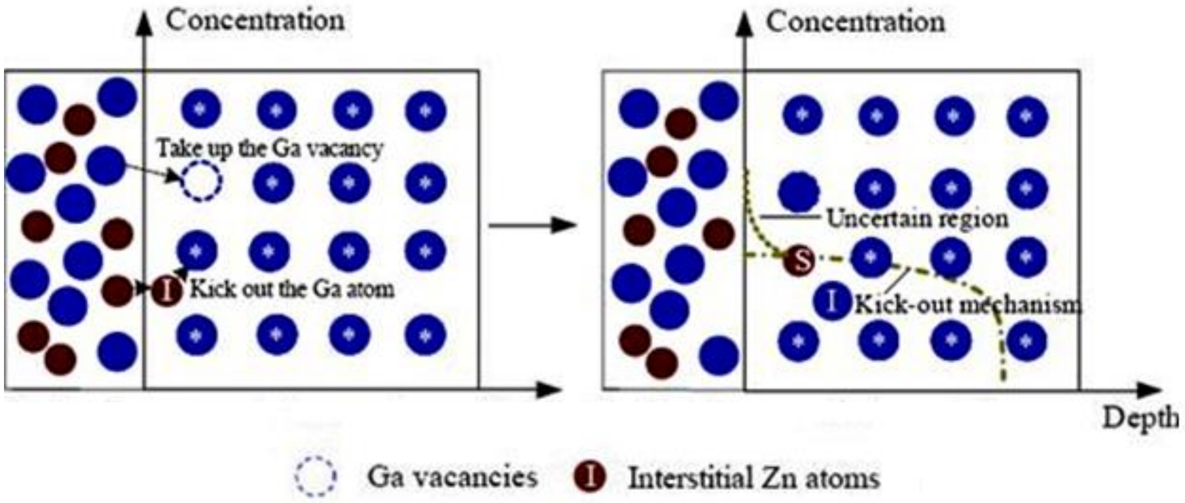
  (1) Native defects, which involve only the atoms of the host crystal, and

  (2) Extrinsic defects, which involve impurity atoms. When an impurity (dopant) is introduced into a pure semiconductor.

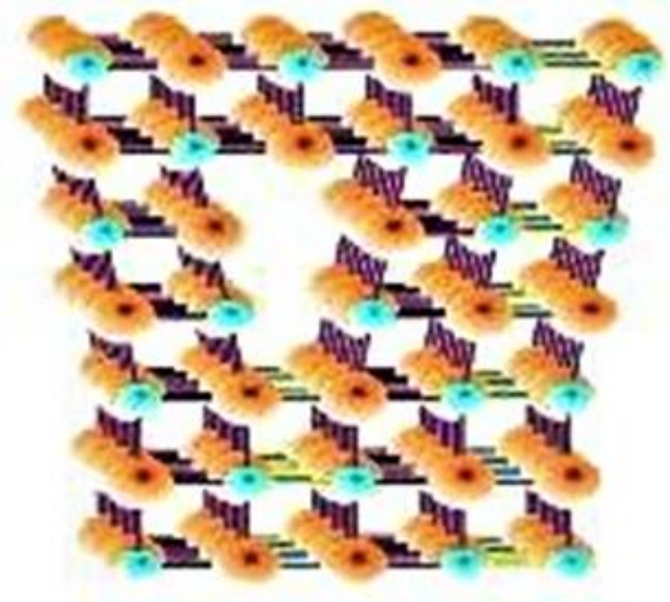
- **Native defects** are due to atomic imperfections in the material. There are ***three types*** of **native** defects: **Vacancies**, **Interstitials**, and **Antisites**.

Vacancies are atomic sites where a host atom in a crystal structure is missing. For example, a gallium vacancy (***V_{Ga}***) in GaAs refers to an imperfection due to a missing **Ga** atom from its site in the crystal lattice



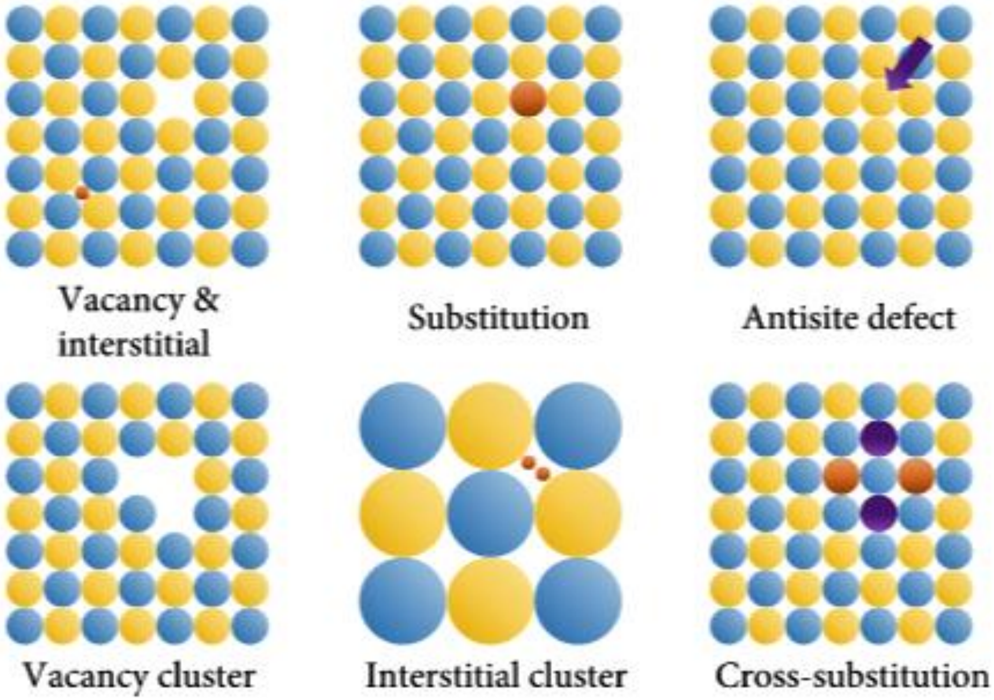


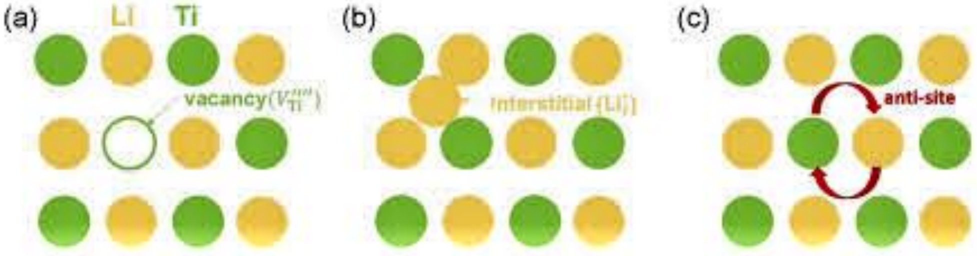
Interstitial defect are when an atom is located in a non-lattice site within the crystal, then it is said to be an 'interstitial'. Interstitial defect are due to host atoms displaced from their regular crystal site. For example, Ga_i refers to a **Ga** atom present inside the unit cell away from its actual atomic site in the crystal.



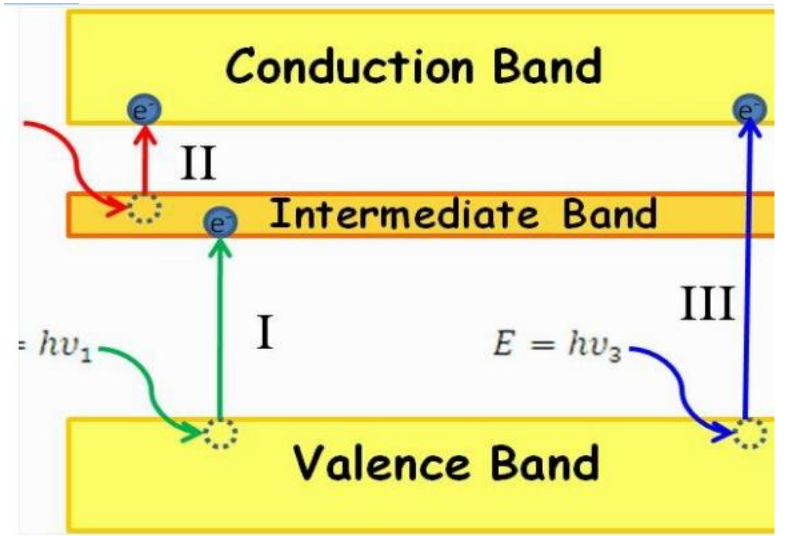
The figure shows how atoms are shifted from their lattice site which in turn resulted in crystal defect

Antisite are atomic sites where the original atomic species has been replaced by another host atom in the crystal. For example, GaAs (gallium antisite) refers to a gallium atom occupying an arsenic site in the crystal.

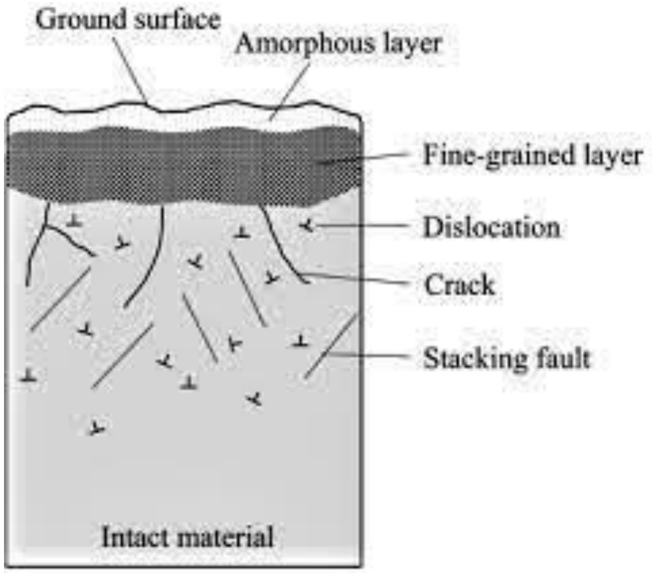




- Defects can create states in the bandgap. These states lead to decreasing the optical energy gap and shifting the absorption edge towards the higher wavelength of the incident photons. Besides, defects behave as traps that affected the motion of the charge carriers.



Another defect might not be related to the material used but with its mechanical integrity. Cracks on the semiconductor which are caused by stresses can make it malfunction.

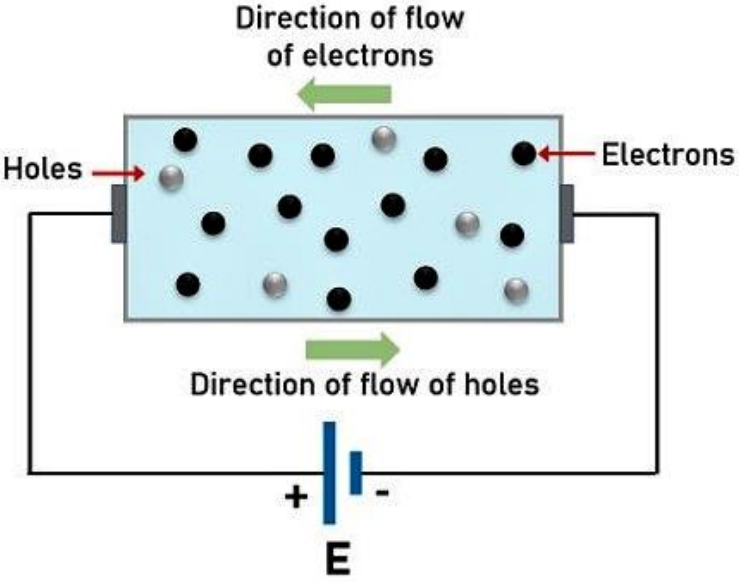


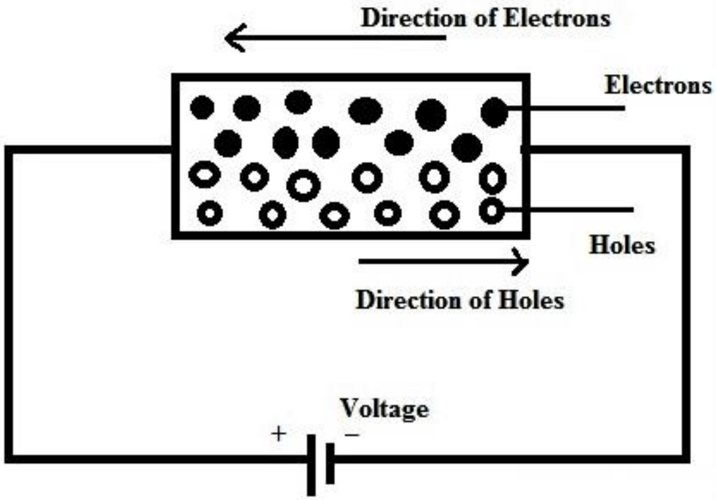
Conduction in semiconductors

Drift current and diffusion current

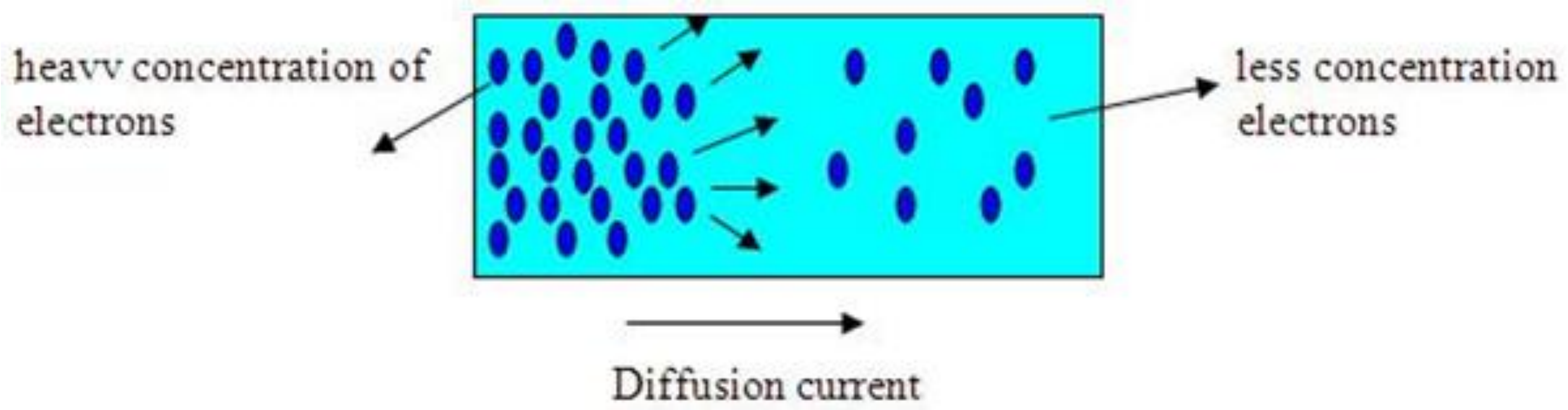
Drift current is the electric current (movement of charge carriers) due to applied electric field. When an electric field is applied across a semiconductor material, a current is produced due to the flow of charge carriers.

Charged particles get pushed by an electric field. Electrons, being negatively charged, get pushed in the opposite direction to the electric field, while holes get pushed in the same direction as the electric field.

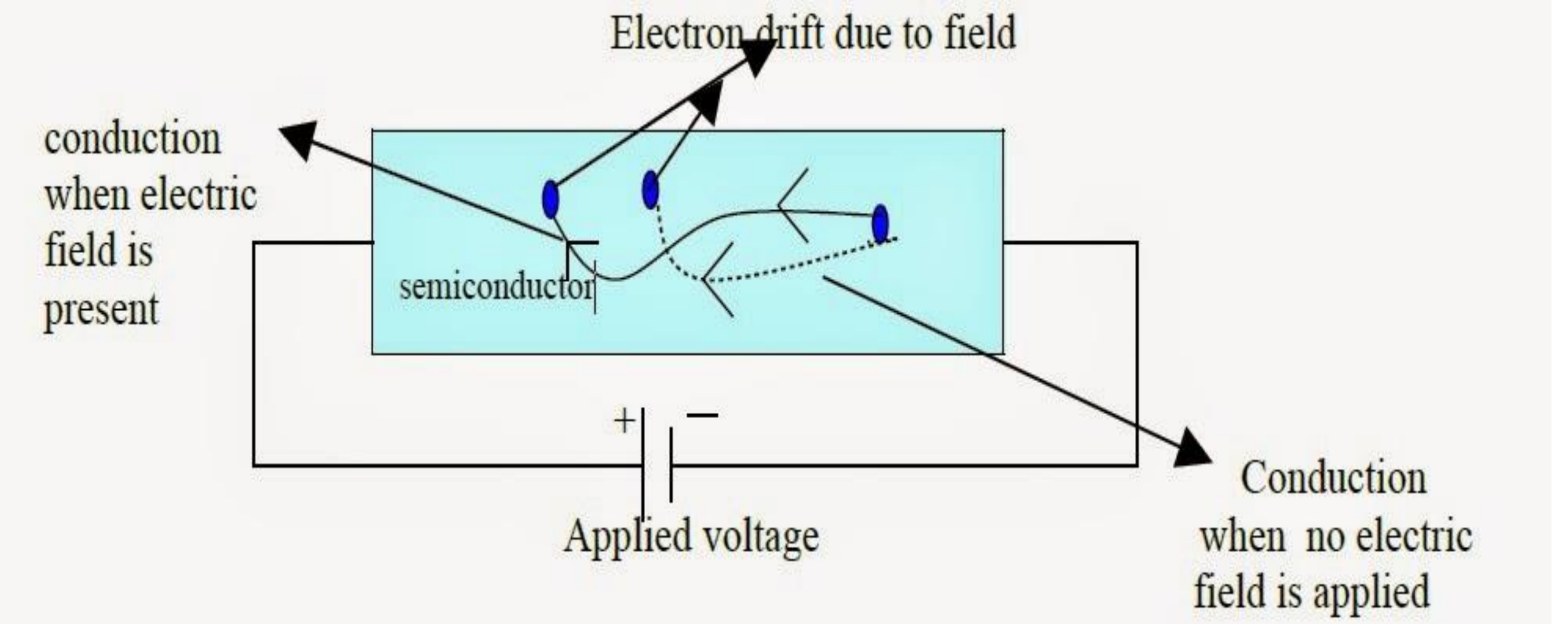




In addition to the drift current, there is a second component of current called the **Diffusion current**. Diffusion is the result of particles undergoing thermal motion. It is the familiar process by which particles move from a point of higher particle density toward a point of lower density. However, drift current is the desired one in semiconductors application.



- Drift current depends on the ability of the carriers to move around in the semiconductor, or the electron and hole mobility. Another parameter drift current depends on is the carrier concentration, because you must have carriers in order to have a current.



Electron and Hole Mobilities

DRIFT

Drift is the motion of charge carriers caused by an electric field. Clearly, drift is usually at play when voltages are applied to a semiconductor device.

Electron and Hole Mobilities: *Consider the velocity*

Carriers have velocities when an electric field is applied to the semiconductor. The drift velocity is so much more important than the thermal velocity in semiconductor devices. The term velocity usually means the ***drift*** velocity.

Electrons and holes move at the thermal velocity are not in a simple straight-line fashion. Their directions of motion change frequently due to **collisions** or scattering in the crystal. The carriers move in a zigzag fashion as shown in Fig. 2–1. ***The mean free time*** between **collisions** is typically 10^{-13} *s* or 0.1 picosecond (ps), and the distance between **collisions** is a few tens of nanometers or a few hundred angstroms. The net thermal velocity is zero. Thus, thermal motion does not create a steady electric current.

Mean free time or **collision** time or conductivity relaxation time ($\boldsymbol{\tau}$) is the average between carriers' **collisions** in a semiconductor. The **mean free path** is the average distance the electron travels between **collisions**.

- It is highly demanded to increase (provide longer) mean free path for charge carriers and at the same time, minimizing collisions between charge carriers so that a steady and useful current can be obtained.

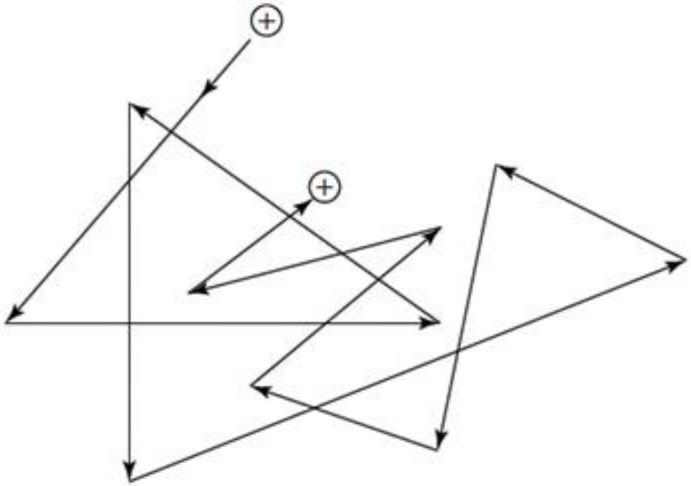


FIGURE 2–1 The thermal motion of an electron or a hole changes direction frequently by scattering off imperfections in the semiconductor crystal.

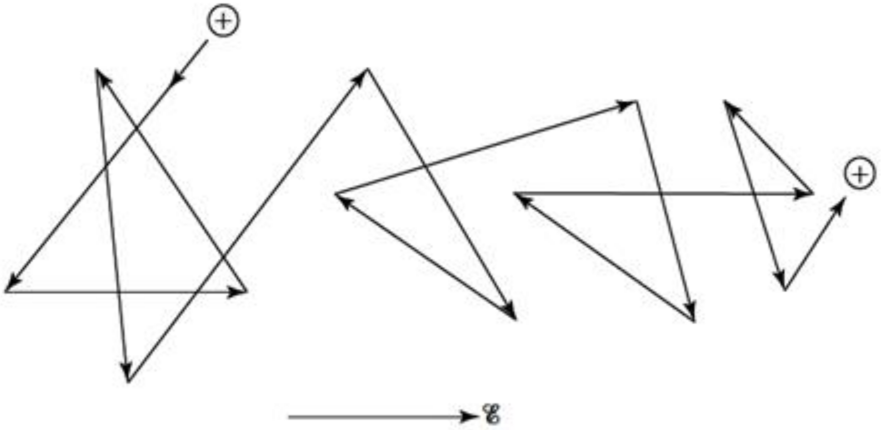


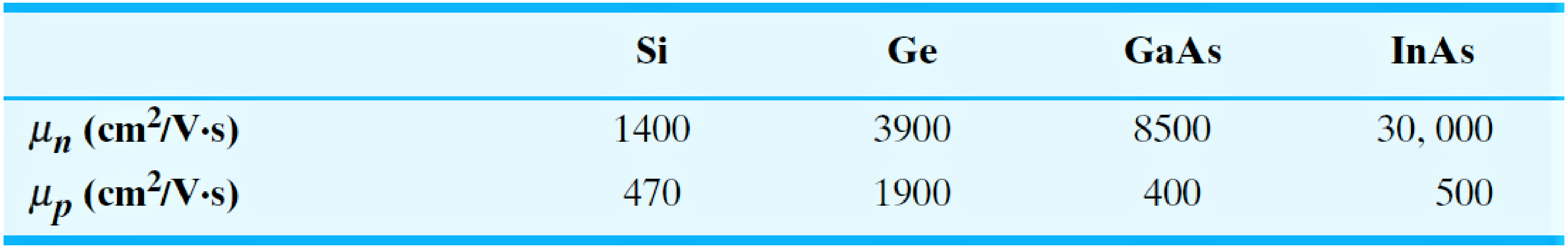
FIGURE 2–2 An electric field creates a drift velocity that is superimposed on the thermal velocity.

- ✓ A faster carrier velocity is desirable, it allows a semiconductor device or circuit to operate at a higher speed.

$$\boxed{v = \mu \, \pounds \ \text{cm}^2/\text{V}\cdot\text{s.}}$$

V: drift velocity
μ: mobility
£: electric field

Electron and hole mobilities at room temperature of selected lightly doped semiconductors.



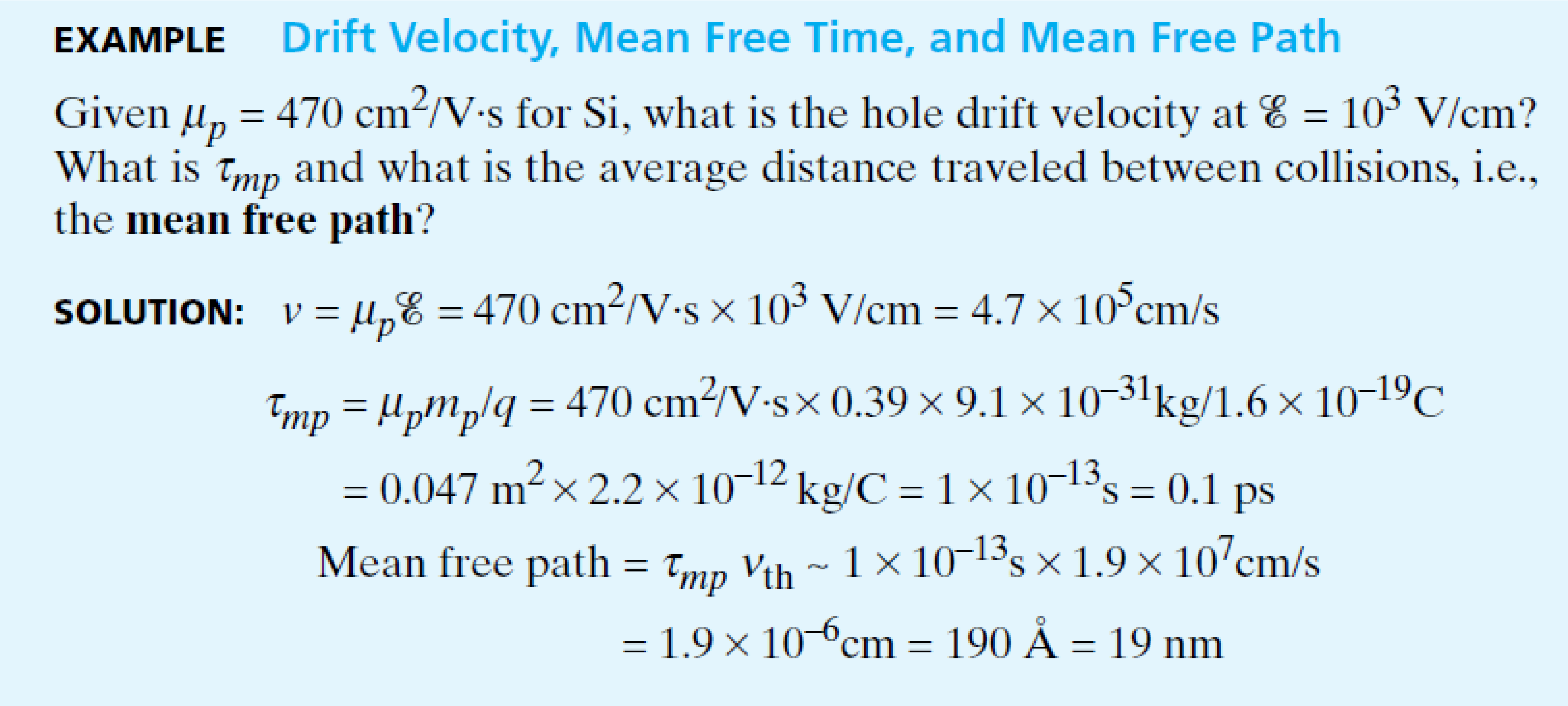
	Si	Ge	GaAs	InAs
μ_n (cm^2/V·s)	1400	3900	8500	30, 000
μ_p (cm^2/V·s)	470	1900	400	500

$v = \mu \pounds$ cm^2/V·s. (*-ve signal*)

V: drift velocity
μ: mobility
$\pounds$: electric field

$$\mu_n = \frac{q\tau_{mn}}{m_n} \qquad \mu_p = \frac{q\tau_{mp}}{m_p}$$

τ_m the mean free time
electron effective mass m_n
hole effective mass m_p



EXAMPLE **Drift Velocity, Mean Free Time, and Mean Free Path**

Given $\mu_p = 470\ \text{cm}^2/\text{V}\cdot\text{s}$ for Si, what is the hole drift velocity at $\mathscr{E} = 10^3$ V/cm? What is τ_{mp} and what is the average distance traveled between collisions, i.e., the **mean free path**?

SOLUTION: $v = \mu_p \mathscr{E} = 470\ \text{cm}^2/\text{V}\cdot\text{s} \times 10^3\ \text{V/cm} = 4.7 \times 10^5 \text{cm/s}$

$$\tau_{mp} = \mu_p m_p/q = 470\ \text{cm}^2/\text{V}\cdot\text{s} \times 0.39 \times 9.1 \times 10^{-31}\text{kg}/1.6 \times 10^{-19}\text{C}$$

$$= 0.047\ \text{m}^2 \times 2.2 \times 10^{-12}\ \text{kg/C} = 1 \times 10^{-13}\text{s} = 0.1\ \text{ps}$$

$$\text{Mean free path} = \tau_{mp}\, v_{\text{th}} \sim 1 \times 10^{-13}\text{s} \times 1.9 \times 10^7\text{cm/s}$$

$$= 1.9 \times 10^{-6}\text{cm} = 190\ \text{Å} = 19\ \text{nm}$$

$q = 1.6 \times 10^{-19}$ C

τ_m the mean free time

m_n electron effective mass

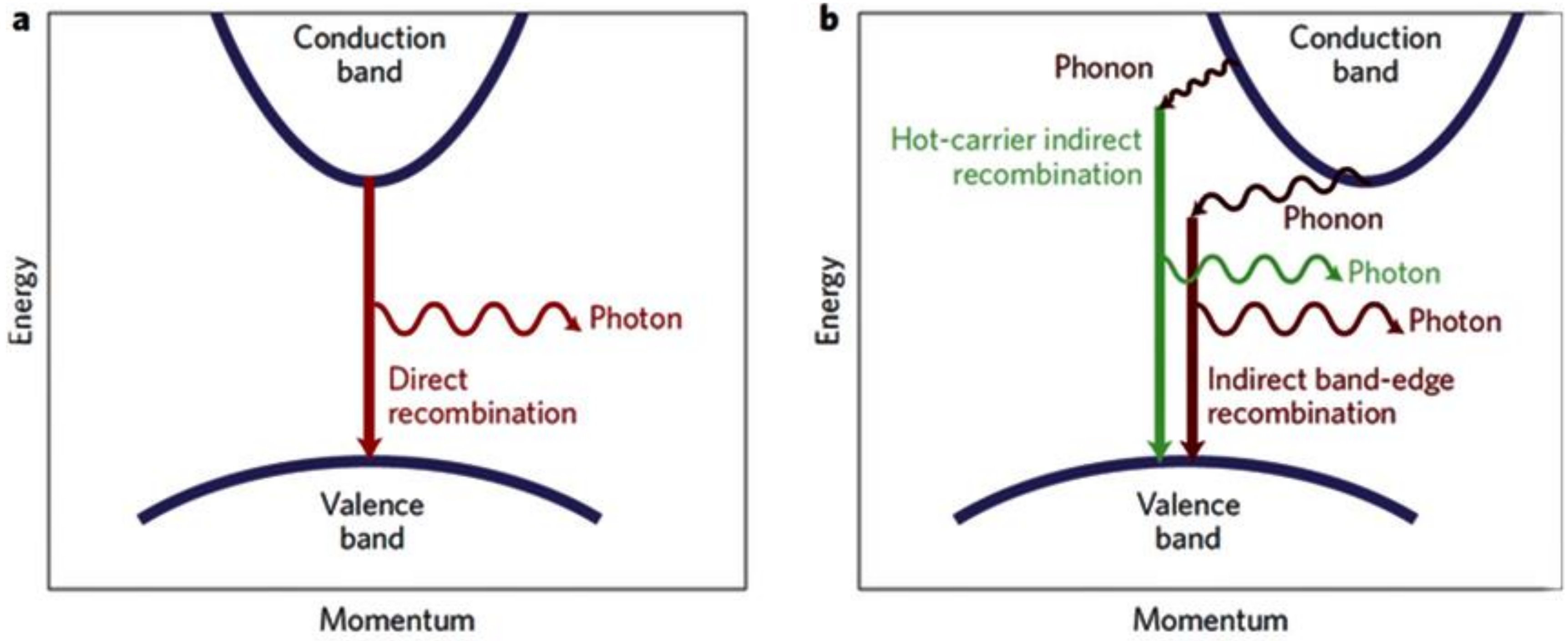
m_p hole effective mass

The effective mass of electrons or holes is (9.11×10^{-31} kg)

Electron-hole recombination

The process in which an **electron**, which has been excited from the valence band to the conduction band of a semiconductor, falls back into an empty state in the valence band, which is known as a hole is known as electron-hole recombination.

An energy approximately equal to the band gap is released in the process of electron-hole recombination. The released energy is called as radiative emission if the released energy is light.



Q1/ Should the mean free path for charge carriers increased? Why and how?

Q2/ define/compare between radiative and non-radiative emission