

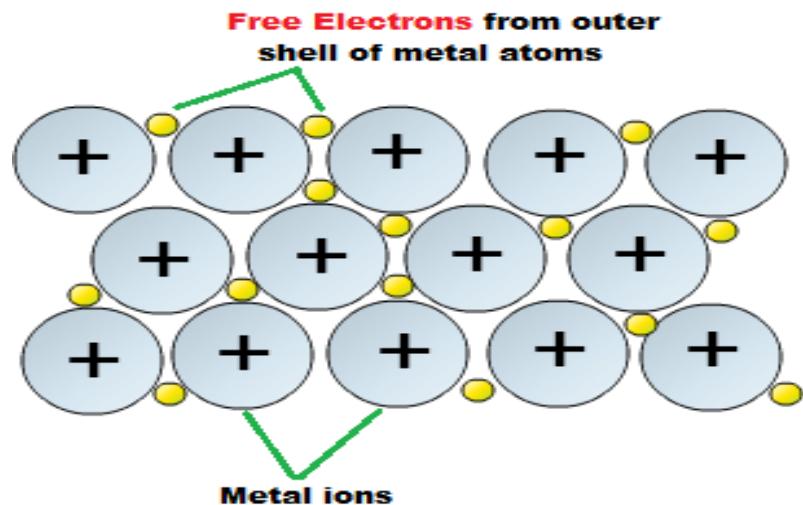
Unit V

Solid State Physics

Free electron theory of Metals

- The treatment of a metal as containing a gas of electrons completely free to move within it.
- The theory was originally proposed in 1900 to describe and correlate the electrical and thermal properties of metals. Later, quantum mechanics became the basis. We can categorize Free Electron Theory as follow:

- 1) Classical free electron theory
- 2) Quantum free electron theory



Classical Free Electron Theory: In 1900 a theory named as Drude –Lorentz of metals explained the classical picture of free electrons in metals. It is based on:

- 1) The valence electrons of atoms are free to move about the whole volume of the metal.
- 2) The collisions of free electrons with other electrons and +ve ions are elastic in nature (no loss in energy)
- 3) The momentum of free electrons vary according to the laws of classical kinetic theory of gases.
- 4) Electrons is in accordance with classical Maxwell-Boltzman distribution
- 5) Under the effect of an electric field, the free electrons get accelerated. However the direction is opposite to that of the direction of the applied electric field.

Failed to explain: Compton Effect, photoelectric effect and black body radiation.

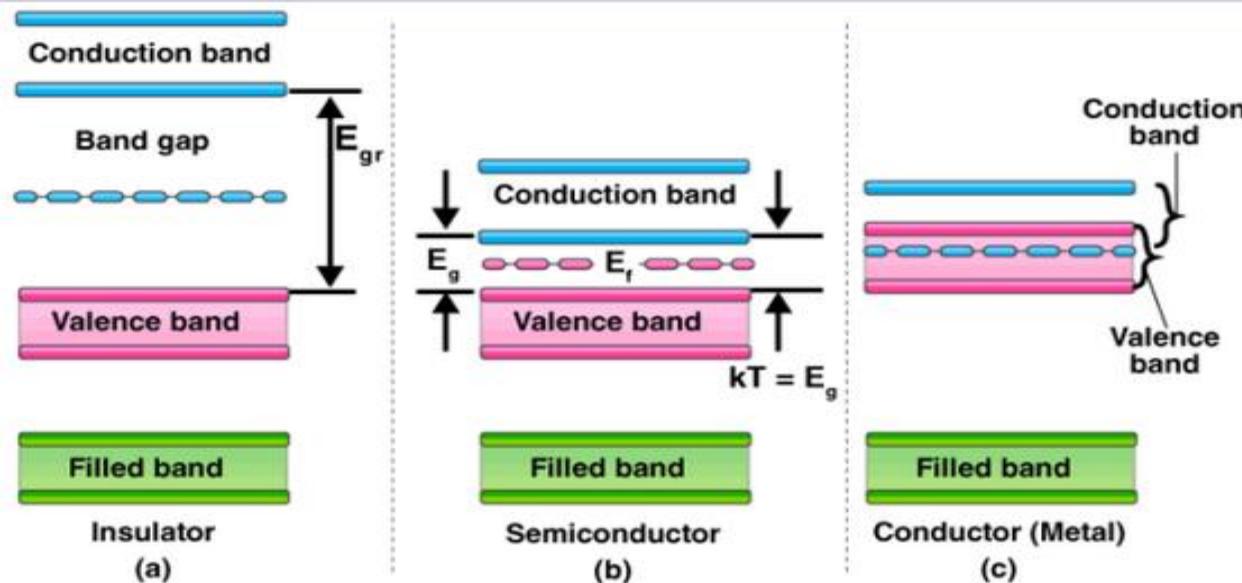
Quantum Free Electron Theory: The Sommerfeld introduced this in 1928. It overcomes drawbacks of the classical theory by applying quantum mechanical principles in 1928.

- 1) Inside the metal electrons can move in a constant potential but remain confined within its boundaries and come out of this potential.
- 2) Free electrons in metal are responsible for electrical conduction. Electrons have quantised energy levels.
- 3) The distribution of electrons in various allowed energy levels is in accordance with Pauli Exclusion Principle.
- 4) Electrons have wave nature so with the help of Fermi-Dirac distribution function Velocity and energy distribution can determine.
- 5) **Attractive forces** between the electrons and the lattice ions as well as the repulsive forces between the electrons themselves are ignored.
- 6) The energy loss: due to interaction of the free electron with the other free electron.

Band Theory in Solid State Physics

- Band theory is a theoretical model explaining the states of electrons of solids is based on the valence band and conduction band.
- It is also known as the band theory of solids or zone theory of solids. It defines conductors, semiconductors and insulators very clearly and distinctly. The energy bands are
- **Valence Band:** that consists of valence electrons energy levels, is known as the valence band. The electrons of this band are loosely bound to the nucleus of the atom.
- **Conduction Band:** beyond valance band the energy level is known as the conduction band. For electrons to be free, external energy must be applied such that the valence electrons get pushed to the conduction band and become free.
- **Forbidden Band:** The energy gap between the valence band and the conduction band is known as the forbidden band

- **Conductors:** electrons jump from valence band to conduction band even at ordinary temperature and if this happens then the solid conducts electricity.
- **Insulator:** If the gap or energy difference between the valence band and conduction band is **more than or equal to 5ev** then the material will behave as an insulator.
- **Semiconductor:** If the energy difference between the valence band and conduction band is equal to or **less than 3ev** then the material or solid is called a semiconductor



Basics for Semiconductors

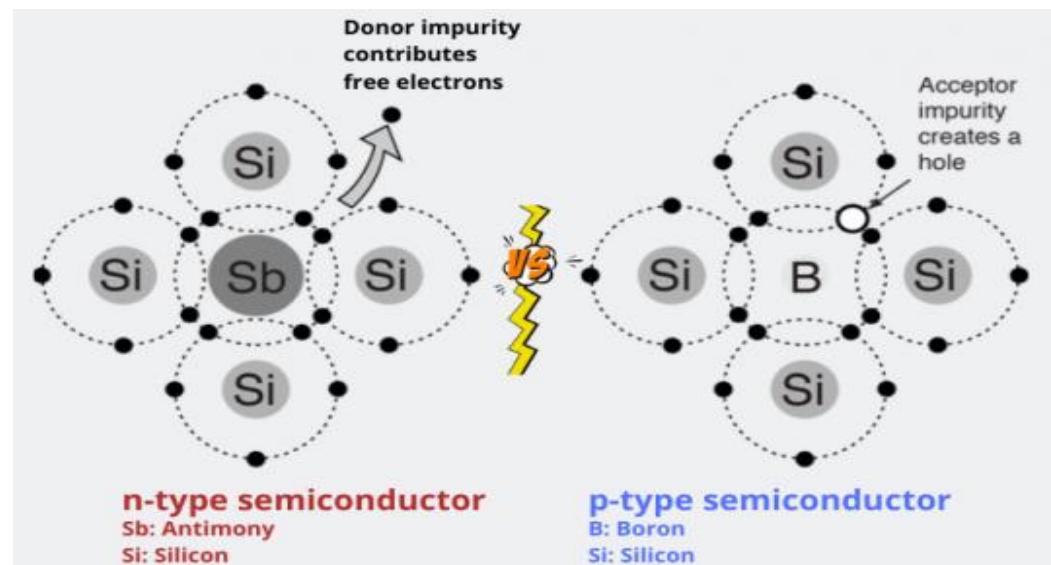
- Semiconductors are materials which have a conductivity between conductors (generally metals) and nonconductors or insulators (such as most ceramics). Semiconductors can be pure elements, such as silicon or germanium, or compounds such as gallium arsenide (GaAs) or cadmium selenide (CdSe).
- In a process called doping, small amounts of impurities are added to pure semiconductors causing large changes in the conductivity of the material.

P-type semiconductor

- Electron minority carriers
- Holes Majority carriers

N-type semiconductor

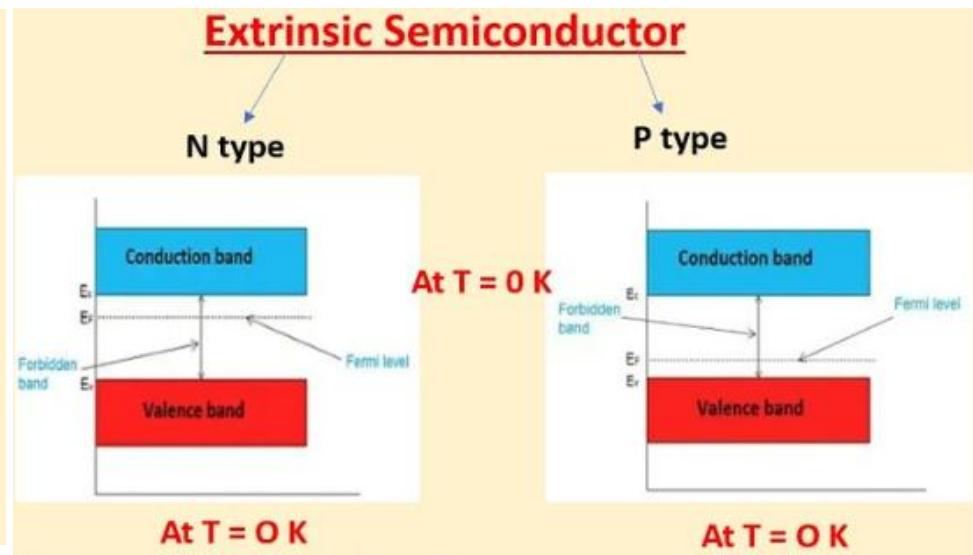
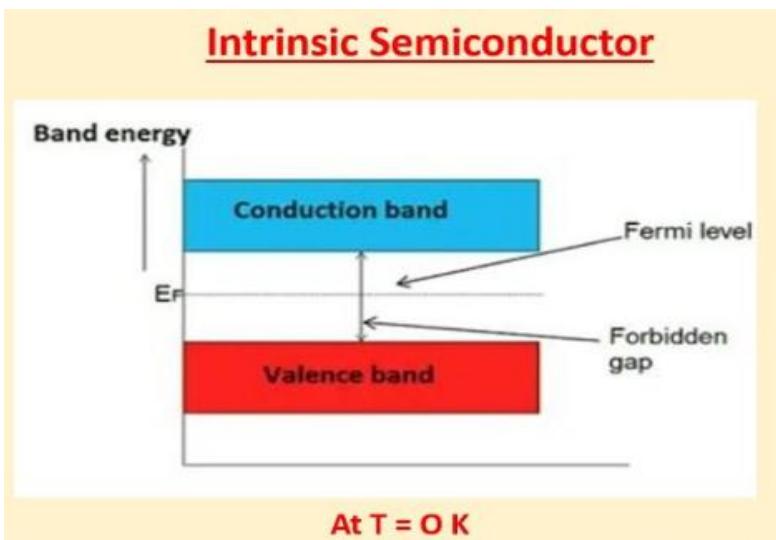
- Electron majority carriers
- Holes minority carriers



Extrinsic semiconductors

The doping of the semiconductors increases its conductivity. The process of deliberately adding a desirable impurity is known as doping and the impurity atoms are called dopants. Extrinsic semiconductors are further classified into two types - N-Type semiconductors and P-type semiconductors.

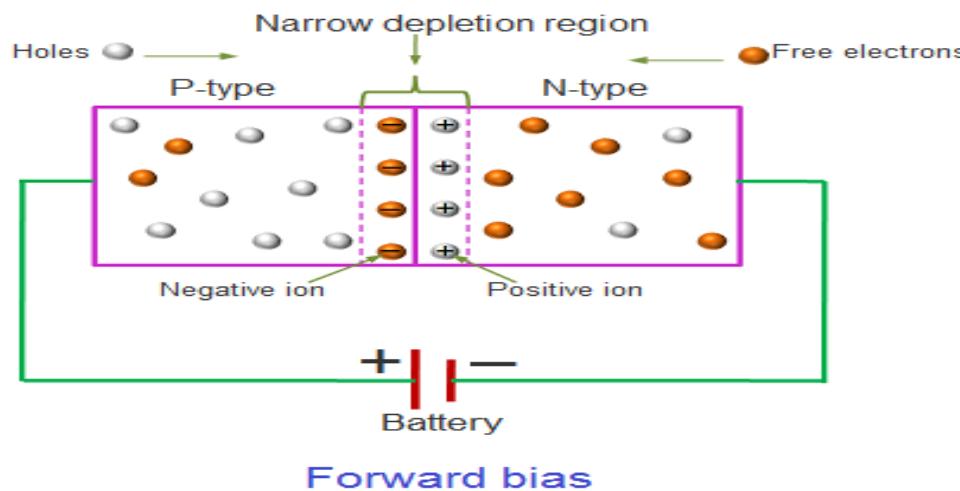
Fermi Level: The highest energy level that an electron can occupy at the absolute zero temperature is known as the Fermi Level. The Fermi level lies between the valence band and conduction band because at absolute zero temperature the electrons are all in the lowest energy state.



P-N Junction Diode

A p-n junction diode is two-terminal or two-electrode semiconductor device, which allows the electric current in only one direction while blocks the electric current in opposite or reverse direction.

Biassing of PN junction: Means connection to the external circuit

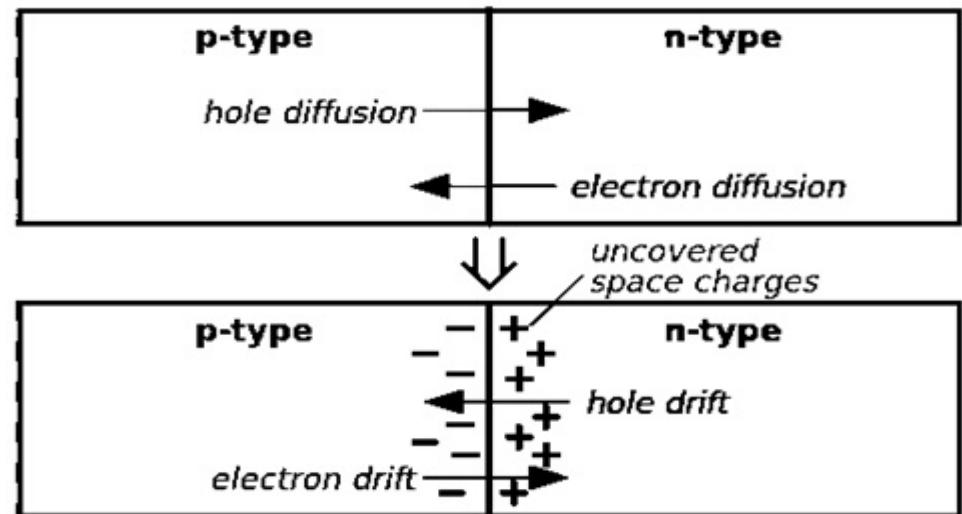


Forward Bias— The voltage potential is connected positively to the P-type terminal and negatively to the N-type terminal of the Diode.

Reverse Bias— The voltage potential is connected negatively to the P-type terminal and positively to the N-type terminal of the Diode.

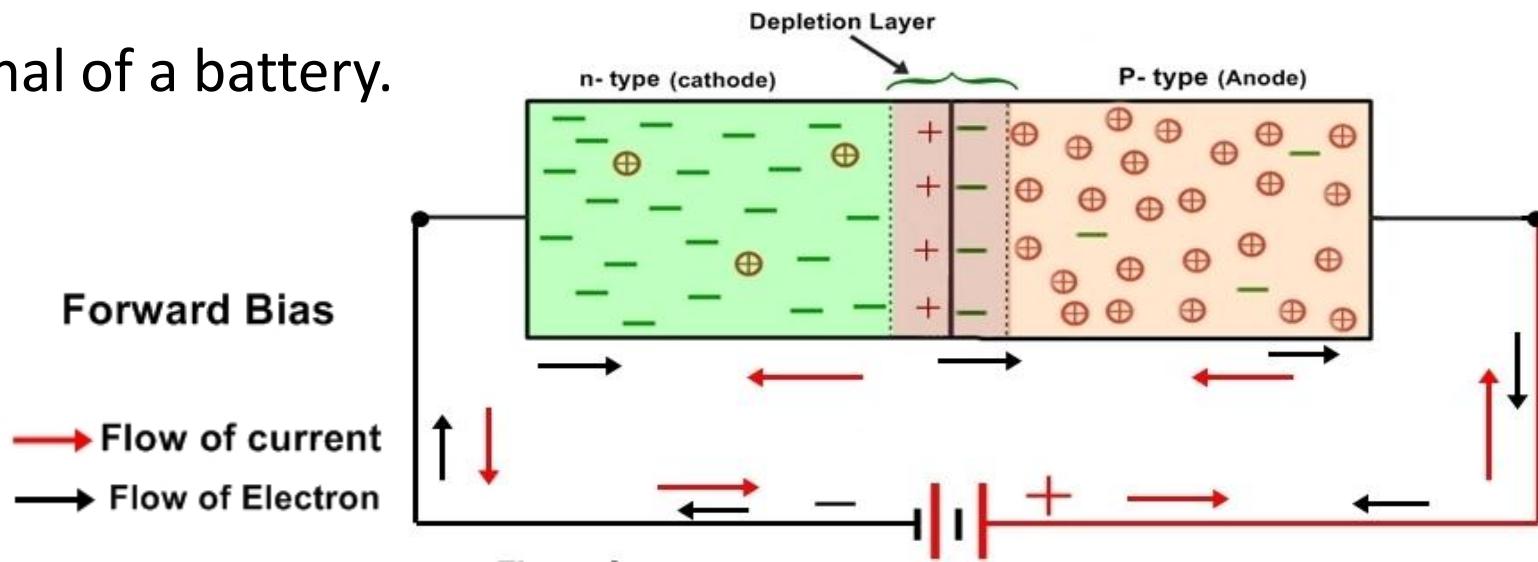
Diffusion Current

- Diffusion current is mainly generated in semiconductors. The doping done in the semiconductors is non-uniform. In order to achieve uniformity, the flow of charge carriers takes place from higher concentration area to lower concentration area.
- The process by which, charge carriers (electrons or holes) in a semiconductor moves from a region of higher concentration to a region of lower concentration is called diffusion.
- Fick's law is applicable on diffusion current which is dependent on gradient of charge density



Drift Current

- The flow of charge carriers, which is due to the applied voltage or electric field is called drift current.
- In a semiconductor, there are two types of charge carriers, they are electrons and holes. When the voltage is applied to a semiconductor, the free electrons move towards the positive terminal of a battery and holes move towards the negative terminal of a battery.



Fermi energy and Fermi-Dirac (F-D) distribution function

- **Fermi energy** is often defined as the highest occupied energy level of a material at absolute zero temperature. In other words, all electrons in a body occupy energy states at or below that body's **Fermi energy at 0K**.
- This concept of Fermi energy is useful for describing and comparing the behavior of different semiconductors. For example: an n-type semiconductor will have a Fermi energy close to the conduction band, whereas a p-type semiconductor will have a Fermi energy close to the valence band.

- The value of the Fermi level at absolute zero (-273.15 °C) is called the Fermi energy and is a constant for each solid. The Fermi level changes as the solid is warmed and as electrons are added to or withdrawn from the solid.
- **What are Fermions:** any member of a group of subatomic particles having odd half-integral angular momentum (J) (spin $\frac{1}{2}$, $\frac{3}{2}$), named for the Fermi-Dirac statistics that describe its behavior (e.g., electrons, muons, neutrons, protons).

Fermions	Bosons
Leptons Quarks	Spin $\frac{1}{2}$ 1
Baryons (qqq)	$\frac{1}{2}, \frac{3}{2}, \dots$ $\frac{5}{2}, \dots$ 0, 1, 2, ...
Mesons (q \bar{q})	Carrier Bosons $\gamma W^+ W^- Z^0 g$

Fermi-Dirac distribution $f(E)$: As a material's temperature rises above absolute zero, we can approximate the *average* energy level at which an electron is present.

$$f(E) = \frac{1}{1 + e^{\left(\frac{E-E_f}{k_B T}\right)}}$$

Here $k(B) = 1.38 \times 10^{-23} \text{ J/K} = 8.625 \times 10^{-5} \text{ eV/K}$

where E is the energy level, k is the Boltzmann constant, T is the (absolute) temperature,

The calculations of Fermi-energy state using are in next slides

$$E_f = \left(\frac{\hbar^2}{8m}\right)\left(\frac{3N}{\pi V}\right)^{\frac{2}{3}}$$

N - number of possible quantum states

V - volume

m - mass of electron

\hbar - planck's constant

Fermi-Dirac distribution function, we are particularly interested in knowing the chance by which we can find a fermion in a particular energy state of an atom. Here, by fermions, we mean the electrons of an atom which are the particles with $\frac{1}{2}$ spin, bound to Pauli exclusion principle.

Let us try to understand the meaning of Fermi level.

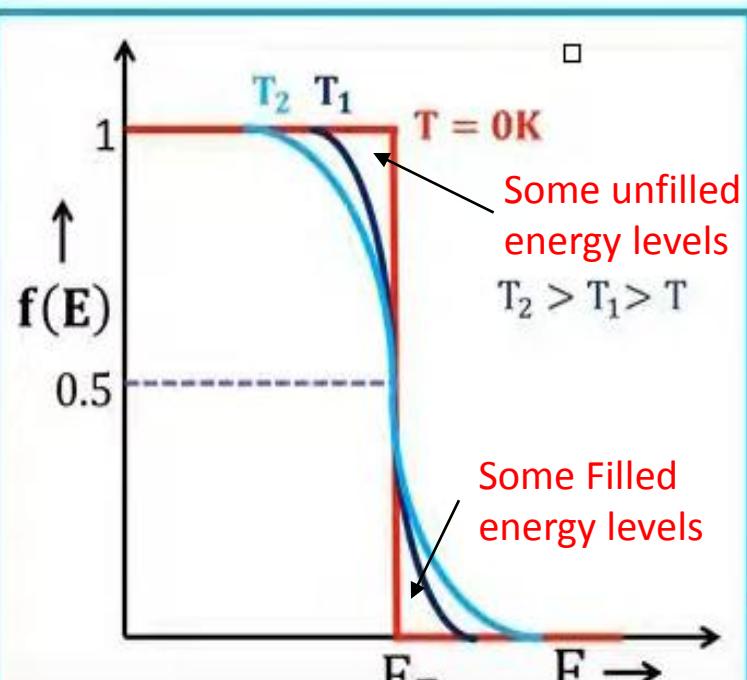
Put $E = E_f$ in $f(E)$

$$f(E) = \frac{1}{1 + e^{\left(\frac{E-E_f}{K_B T}\right)}}$$

$$\begin{aligned} f(E) &= \frac{1}{1 + e^{\left(\frac{E_f - E_f}{K_B T}\right)}} = \frac{1}{1 + e^0} \\ &= \frac{1}{1 + 1} = \frac{1}{2} \end{aligned}$$

This means the Fermi level is the level at which one can expect the electron to be **present exactly 50%**.

Fermi-Dirac Distribution Function at various temperatures



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

At $T = 0\text{ K}$, For $E < E_F$

$$e^{\left(\frac{E-E_F}{kT}\right)} = e^{\frac{-\text{ve number}}{0}} = e^{-\infty} = \frac{1}{e^{\infty}} = \frac{1}{\infty} = 0$$

$$\therefore f(E) = \frac{1}{1 + e^{\left(\frac{E-E_F}{kT}\right)}} = \frac{1}{1 + 0} = 1$$

This indicates all energy levels below E_F are completely filled at absolute zero temperature

At $T = 0\text{ K}$, For $E > E_F$

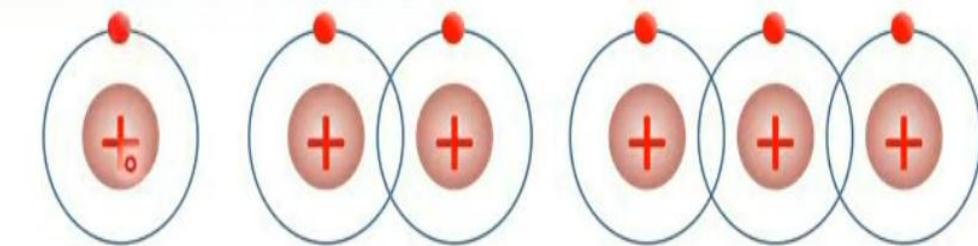
$$e^{\left(\frac{E-E_F}{kT}\right)} = e^{\frac{+\text{ve number}}{0}} = e^{+\infty} = \infty$$

$$\therefore f(E) = \frac{1}{1 + e^{\left(\frac{E-E_F}{kT}\right)}} = \frac{1}{1 + \infty} = 0$$

This indicates all the energy levels above Fermi energy are completely empty at 0K

Formation of Bands

- An isolated atom of a metal possesses discrete energies of different electrons.
- When two single or isolated atoms are bring close to each other (decreasing interatomic distance) then the outermost orbit electrons of two atoms are interact with each other. i.e, the electrons in the outermost orbit of one atom experience a attractive force from the nearest or neighboring atomic nucleus.
- Due to this the **energies of the electrons will not be in same level**, the energy levels of electrons are changed to a value which is higher or lower than that of the original energy level of the electron.

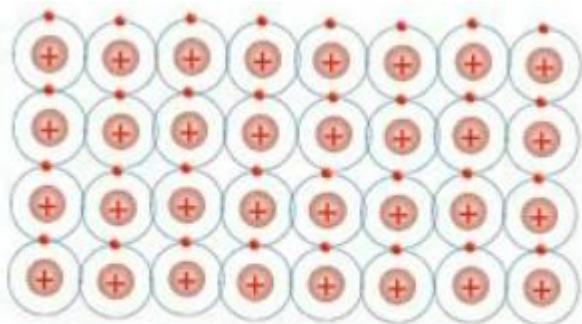


Showing the interaction of two and three electrons and their corresponding energies

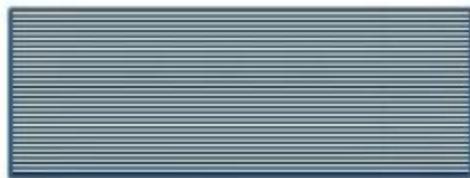
$$E_1 \text{ ---}$$

$$E_1 \text{ ---}$$

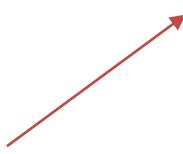
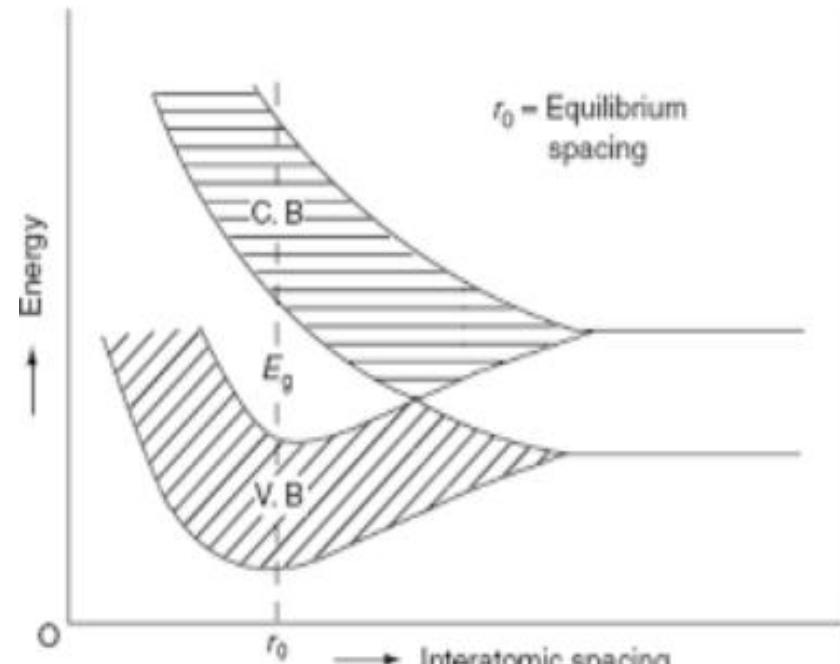
$$\begin{array}{c} E_1 \\ E_2 \\ E_3 \end{array} \text{ ---}$$



N-atoms



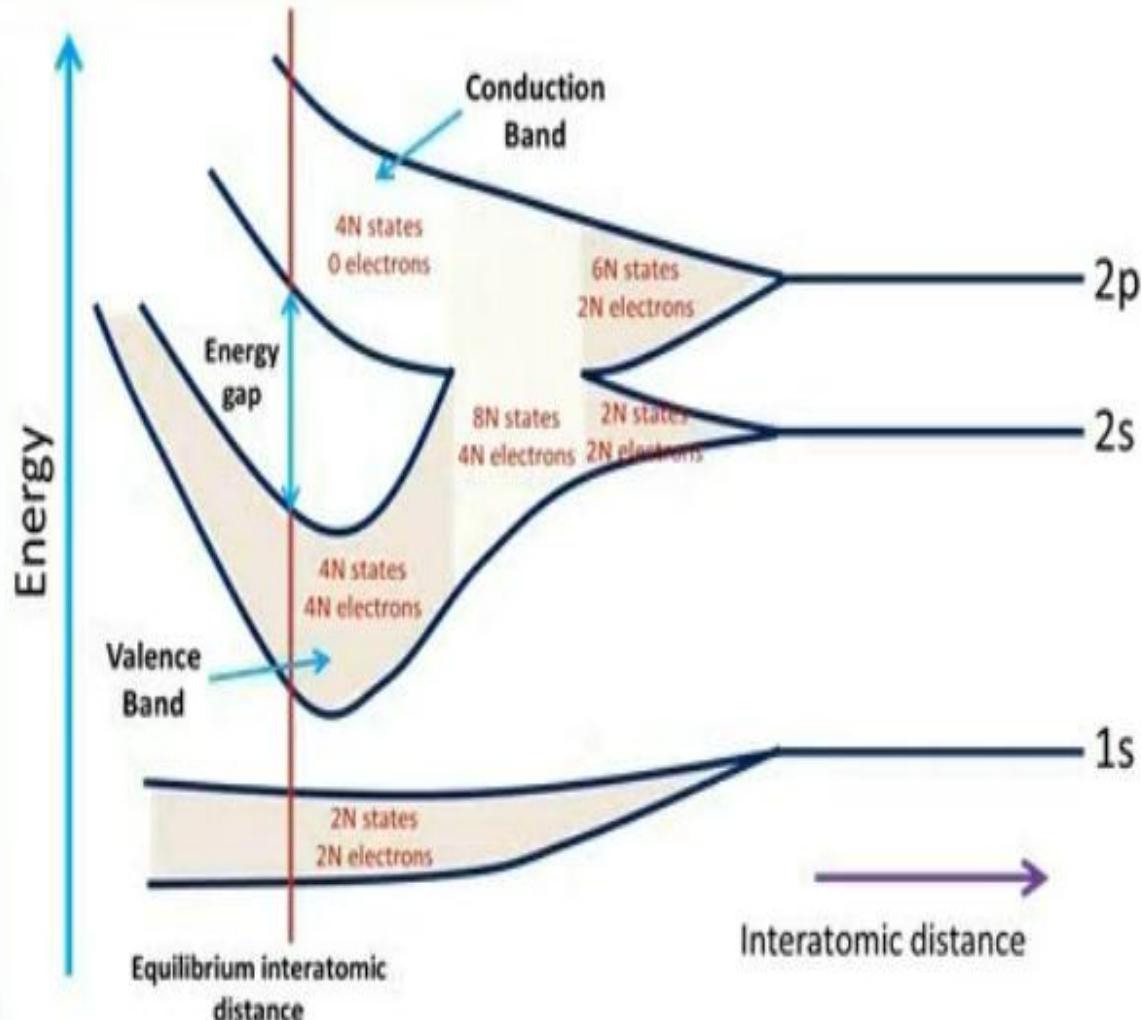
N-levels



As the N-atoms are pushing towards (up to equilibrium interatomic distance) each other means we are decreasing the interatomic distance.

Example of Carbon Atoms

- Electronic structure
individual carbon atom:
 $1s^2 2s^2 2p^2$
- Each atom has two $1s$ states, two $2s$ states, six $2p$ states and the higher states.
- Hence for N atoms, there will be $2N$, $2N$ and $6N$ available states of type $1s$, $2s$, and $2p$ respectively.

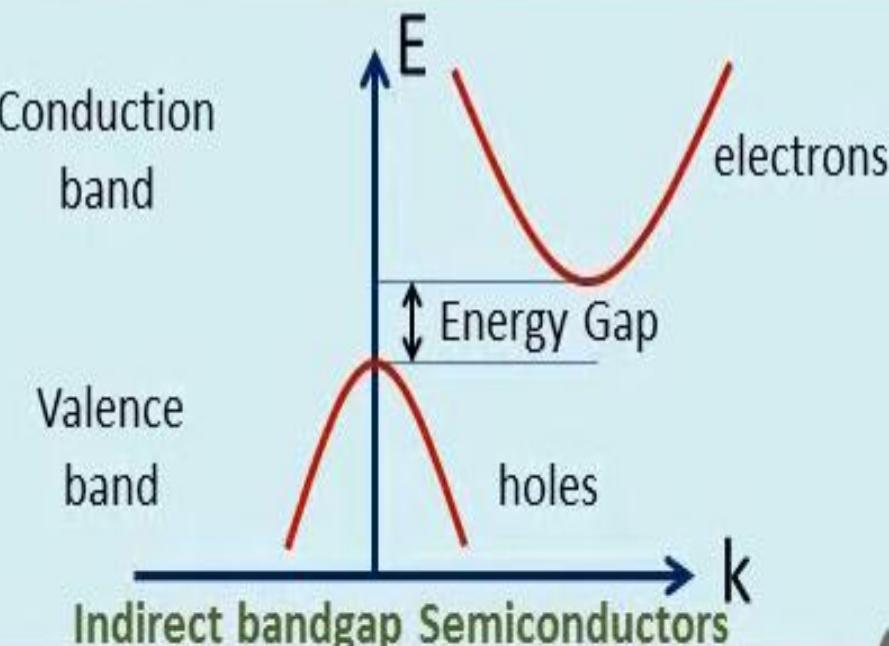
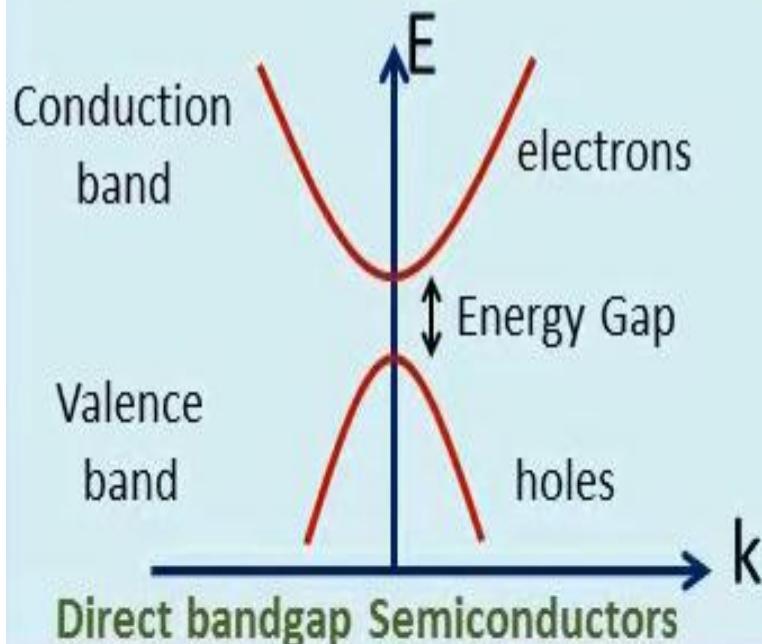


By using Aufbau principle: It states that electrons are filled into atomic orbitals in the increasing order of orbital energy level.

Direct Gap and Indirect Gap Semiconductors

The energy of an electron is given by $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$ where p is momentum, m is mass of an electron, \hbar is Planck's constant and k is propagation constant

Thus $E \propto k^2$ which is an equation of parabola. The graph of E vs k is shown below -

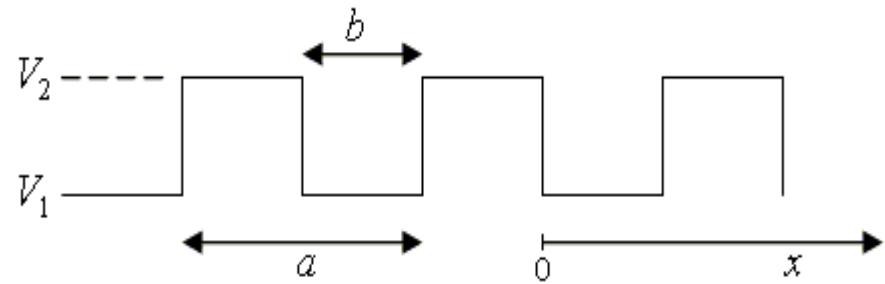
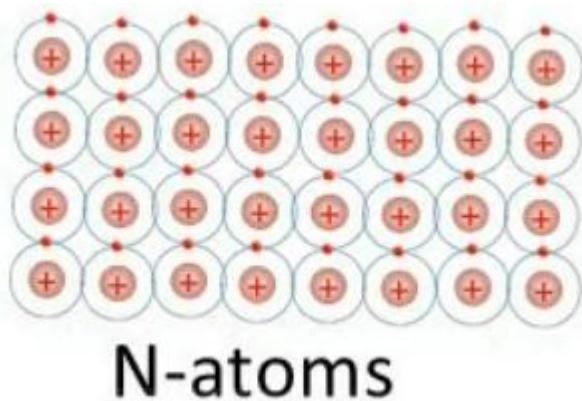


- In direct band gap semiconductor, the bottom of the conduction band and top of the valence band lies at the same value of K . In this, electron can directly excite or de-excite by the absorption or emission of photon and there is no phonon involvement in the process of excitation and de-excitation.
- Direct bandgap semiconductors are used in light-emitting applications like LED and LASER. Ex. GaAs, CdS, ZnS, CdSe etc.
- In Indirect band gap semiconductor, top of the valence band and bottom of the conduction band lies at different values of K . If an electron goes from the top of the valence band to the bottom of the conduction band, it has to change its energy as well as wave-vector K .

- For momentum and energy conservation, there is the **involvement of phonon** in the conservation process. If there is de-excitation of the electron, then not all the energy will be emitted in the form of the photon but some energy is emitted in the form of phonons i.e. some part is transferred to the lattice, and the lattice will vibrate and generate heat.
- So indirect bandgap semiconductor bandgap semiconductor **is not suitable for light emission**. Ex. Si, Ge, GaP SiC, etc.
- Note: A phonon is a **definite discrete unit or quantum of vibrational mechanical energy**, just as a photon is a quantum of electromagnetic or light energy.

Effective mass/-ve effective mass electrons

- An electron in crystal may behave as if it had a mass different from the free electron mass m_0 . There are crystals in which the effective mass of the carriers is much larger or much smaller than m_0 . The effective mass may be anisotropic, and it may even be negative.
- The important point is that the electron in a periodic potential is accelerated relative to the lattice in an applied electric as if its mass is equal to an effective mass.



Potential profile for Kronig-Penney model

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \quad (1)$$

$$m = \frac{p^2}{2E} = \frac{\hbar^2 k^2}{2E}$$

Differentiate (1) w.r.t. k

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m} \quad \text{It represents how energy changes with k}$$

Again differentiate above eq. w.r.t. k

$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m} \rightarrow m = \frac{\hbar^2}{\frac{d^2E}{dk^2}} \rightarrow m = m^* = \hbar^2 \left(\frac{d^2E}{dk^2} \right)^{-1}$$

- The effective mass is represented with m^* to distinguish from rest mass
- Effective mass will be +ve, -ve, zero or infinite depending on $\frac{d^2E}{dk^2}$

1. The Fermi level for potassium is 2.1eV. Calculate the velocity of the electron at the Fermi level.

Solution:- We have the formula,

$$E_F = \frac{1}{2}mv_F^2$$

$$\text{Therefore, } v_F = \left(\frac{2E_F}{m}\right)^{\frac{1}{2}}$$

$$= \left[\frac{2 \times 2.1\text{eV} \times 1.602 \times 10^{-19}\text{J/eV}}{9.11 \times 10^{-31}\text{kg}} \right]^{\frac{1}{2}}$$

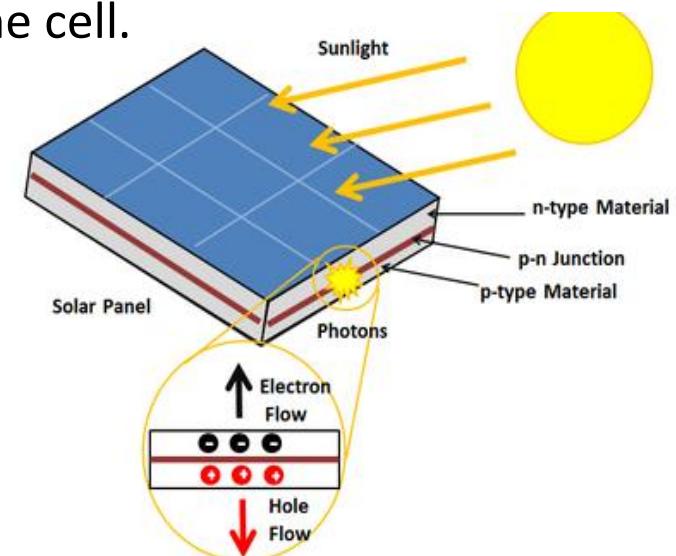
$$v_F = 8.6 \times (10)^5 \text{m/s.}$$

Solar Cell/Photovoltaic Solar Cell

- Solar cells, also called photovoltaic cells, convert the energy of light into electrical energy using the photovoltaic effect.
- It is a form of photoelectric cell, defined as a device whose electrical characteristics, such as current, voltage, or resistance, vary when exposed to light.
- Domestic solar systems convert around 20% of the sunlight converts into electricity, while more expensive commercial systems can convert up to 40%. However, with technological advances the solar efficiency of these panels is expected to rise.



- Solar cells can be arranged into large groupings called arrays. These arrays, composed of many thousands of individual cells
- Silicon is, by far, the most common semiconductor material used in solar cells. And cadmium telluride (CdTe) and copper indium gallium diselenide (CIGS)
- When sunlight shines on the cell, photons (light particles) bombard the upper surface.
- The photons carry their energy down through the cell.
- The photons give up their energy to electrons in the lower, p-type layer.
- The electrons use this energy to jump across the barrier into the upper, n-type layer and escape out into the circuit.



THANK YOU.....