



**DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY**

**18PY103J – Physics: Semiconductor Physics
Module-I, Lecture-1**

**Introduction to Classical Free Electron Theory
& Quantum Free Electron Theory**



Why semiconductors?

- **SEMICONDUCTORS: They are here, there, and everywhere**
- Computers, palm pilots, Silicon (Si) MOSFETs, ICs, CMOS laptops, anything “intelligent”
- Cell phones, pagers Si ICs, GaAs FETs, BJTs
- CD players AlGaAs and InGaP laser diodes, Si photodiodes
- TV remotes, mobile terminals Light emitting diodes (LEDs)
- Satellite dishes InGaAs MMICs (Monolithic Microwave ICs)
- Fiber networks InGaAsP laser diodes, pin photodiodes
- Traffic signals, car taillights GaN LEDs (**green, blue**)
InGaAsP LEDs (**red, amber**)
- Air bags Si MEMs, Si ICs
- and, they are important, especially to Elec.Eng.& Computer Sciences



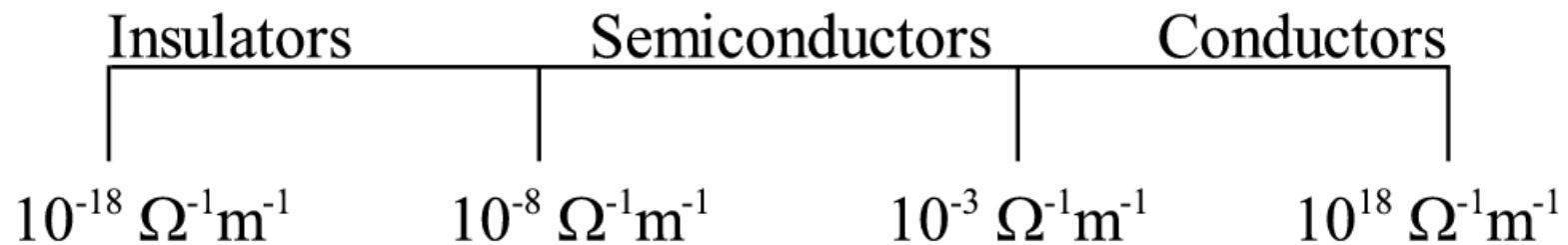
Introduction

Semiconductors are materials whose electrical properties lie between Conductors and Insulators.

Ex : Silicon and Germanium

Give the examples of Conductors and Insulators!

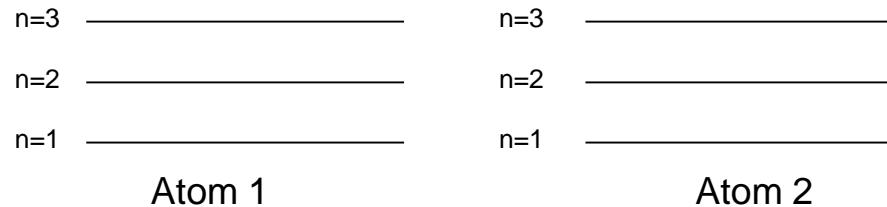
Difference in conductivity



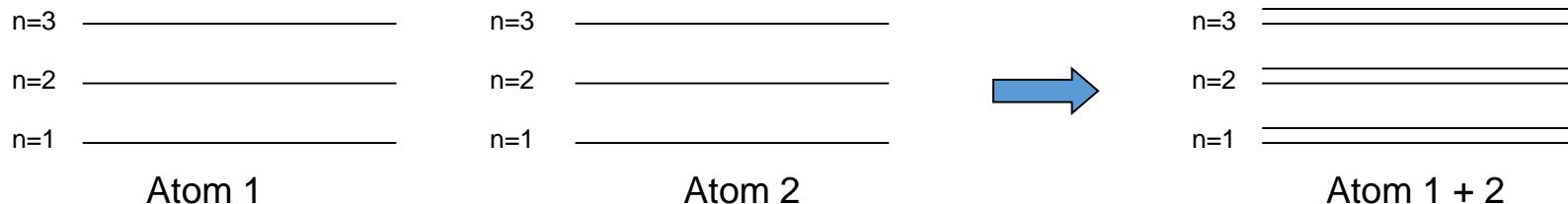


Band theory of a solid

- A solid is formed by bringing together isolated single atoms.
- Consider the combination of two atoms. If the atoms are far apart there is no interaction between them and the energy levels are the same for each atom. The numbers of levels at a particular energy is simply doubled



- If the atoms are close together the electron wave functions will overlap and the energy levels are shifted with respect to each other.





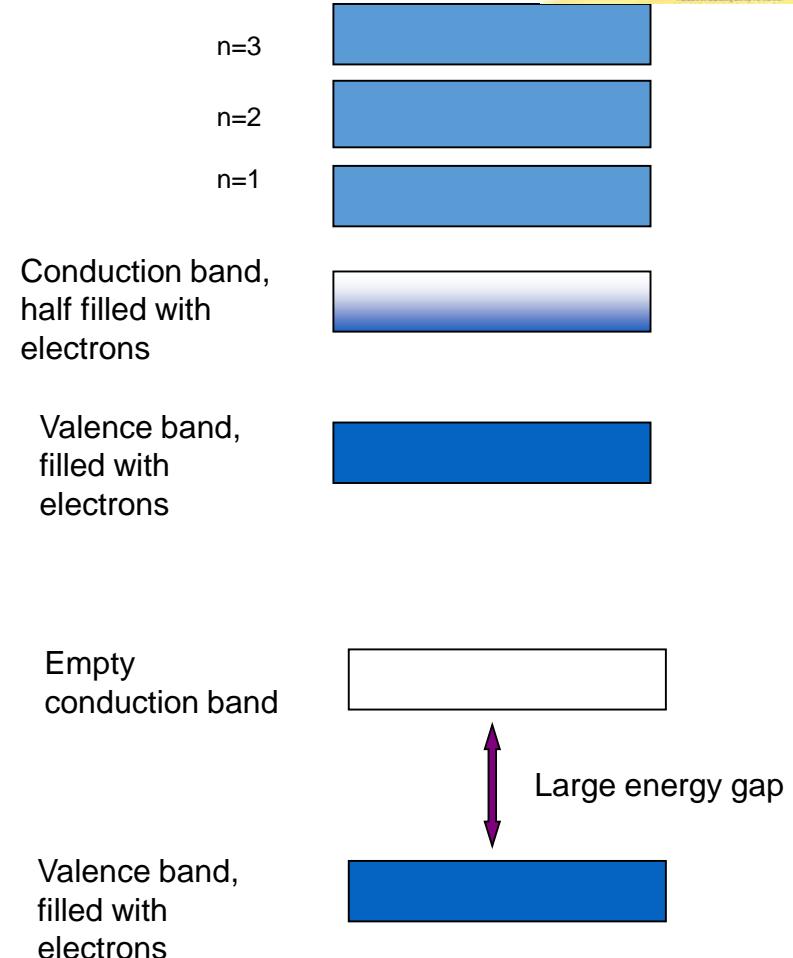
- A solid will have millions of atoms close together in a lattice so these energy levels will creates bands each separated by a gap.

- **Conductors:**

- If we have used up all the electrons available and a band is still only half filled, the solid is said to be a good conductor. The half filled band is known as the conduction band.

- **Insulators:**

- If, when we have used up all the electrons the highest band is full and the next one is empty with a large gap between the two bands, the material is said to be a good insulator. The highest filled band is known as the valence band while the empty next band is known as the conduction band.

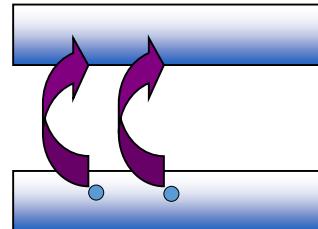




Semiconductors:

- Some materials have a filled valence band just like insulators but a small gap to the conduction band.
- At zero Kelvin the material behave just like an insulator but at room temperature, it is possible for some electrons to acquire the energy to jump up to the conduction band. The electrons move easily through this conduction band under the application of an electric field. This is an **intrinsic semiconductor**.

Conduction band, with some electrons

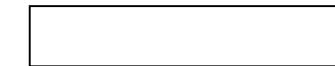


Top valence band now missing some electrons



At room temperature – some conduction

Empty conduction band



Small energy gap



Valence bands, filled with electrons



At zero Kelvin – no conduction

So where are all these materials to be found in the periodic table ?

INTRODUCTION



- Conducting materials are low resistivity materials.
- They conduct heat and electricity effectively.
- A conductor (metal) is a collection of positive ions fixed at their position and a large number of free electrons moving freely anywhere in the conductor.
- Therefore the electrical conductivity depends on the number of free electrons available.
- The thermal conductivity depends on the availability of phonons also.

BASICS TERMINOLOGIES



- **Bounded Electrons:** Valence electrons in isolated atoms bound to their parent nuclei are bounded electrons.
- **Free electrons:** In a solid many atoms are present whose boundaries overlap. Hence the valence electrons find continuity to move and are termed free electrons.
- **Free electron gas:** Collection of free electrons is termed as free electron gas. It is charged.

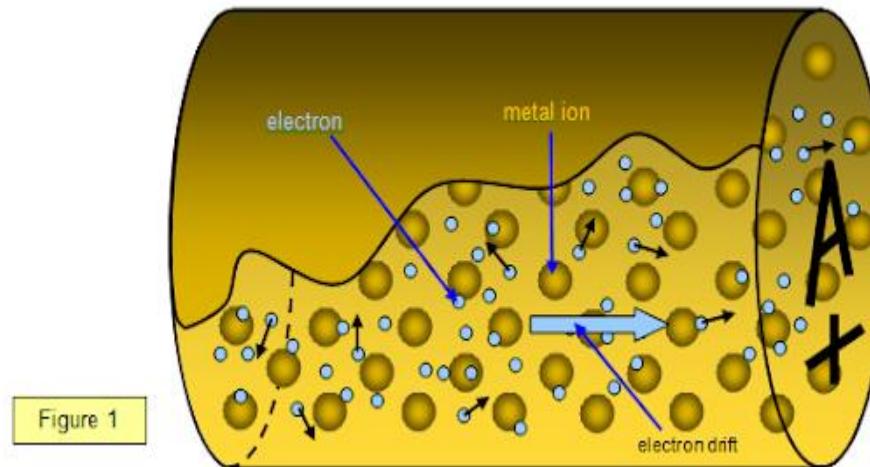


Figure 1



- ***Electric Field (E)***: It is defined as potential drop (V) per unit length (l).
- ***Current density (J)***: Current flowing through a solid per unit area is current density.
- ***Drift Velocity (v_d)***: The average velocity acquired by the free electron in a particular direction, due to the application of electric field.
- ***Mobility (μ)***: Drift velocity acquired by the free electron per unit electric field applied to it is mobility.



- *Relaxation Time (τ)*: Relaxation time can be defined as the time taken for the drift velocity of the electron to decay to $1/e$ of its initial value.
- *Collision Time (τ_c)*: The average time taken by the free electron between two successive collisions is known as collision time.
- *Mean Free Path (λ)* : The average distance travelled by an electron between two successive collisions in the presence of an applied field is known as mean free path.

- Classical Free electron theory:
 - Year: 1900 | Developers: Drude and Lorentz
 - Metals contain free electrons
 - They obey laws of classical mechanics.
- Quantum Free electron theory:
 - Year: 1920 | Developer: Sommerfield
 - Free electrons obey quantum laws and move in a constant potential.
- Zone theory (Brillouin/ Band theory)
 - Year: 1928 | Developer: Bloch
 - Free electrons move in a periodic potential provided by the lattice. Explains semiconductivity based on bands



Free Electron Theory

- The electron theory of materials is to explain the structure and properties of solids through their electronic structure.
- It also gives information about bonding in solids, energy levels in metals and cohesive & repulsive forces in metals.

Development of Free Electron Theory

► The Classical free electron theory [Drude and Lorentz]

It is a macroscopic theory, through which free electrons in lattice and it obeys the laws of classical mechanics. Here the electrons are assumed to move in a constant potential.



► **The Quantum free electron theory [Sommerfeld Theory]**

It is a microscopic theory, according to this theory the electrons in lattice moves in a constant potential and it obeys law of quantum mechanics.

► **Brillouin Zone Theory [Band Theory]**

Bloch developed this theory in which the electrons move in a periodic potential provided by periodicity of crystal lattice. It explains the mechanisms of conductivity, semiconductivity on the basis of energy bands and hence band theory.

The Classical Free Electron Theory

According to kinetic theory of gases in a metal, Drude assumed free electrons are as a gas of electrons.



Drude Theory

This theory initially proposed by Drude in 1900, and it's the first theory to explain the electrical conduction in conducting materials and reveals that free electrons are responsible for the electrical conduction.

Free electrons

In certain metals especially in Cu, Ag and Al valence electrons are so weakly attached to the nuclei they can be easily removed or detached such electrons are called as free electrons.

But all the valence electrons in the metals are not free electrons.

Concept of Classical Free electron Theory

- According to this theory, metals consists of positive ions fixed in lattice and negative ions vander freely within the boundaries of the metal.
- As they are responsible for conductivity called as Conduction electrons
- This cloud of free electrons are called as electron gas
- They differ fro ordinary gas in two aspects
 1. Free electron gas is charged while molecules of ordinary gases are neutral
 2. Concentration of electron is > ordinary gas concentration



Classical Free Electron Theory of Metals

Lorentz in 1900, suggested that free electrons are treated as perfect gas. He used Maxwell-Boltzmann statistics to the electron gas with following assumptions:

1. Mutual repulsion between the negatively charged electrons are neglected
2. Potential field due to positive ions within the crystal is assumed to be constant everywhere.

Electrons motion in the absence of electric field:

1. Possess elastic collision
2. Net displacement in any direction is zero
3. The neglect of electron-electron interaction between collisions is known as the “*independent electron approximation*”



Classical Free Electron Theory of Metals

Electrons motion in presence of electric field:

1. In presence of electric field the equilibrium condition disturbed and the free electrons acquire some energy from electric field.
2. The electrons cannot be accelerated indefinitely due to the collisions of electrons with lattice ions.

3. Drift:

The net movement of electrons due to an applied electric field is called drift.

4. Drift velocity

In the presence of externally applied electromagnetic fields, the electrons acquire some amount of energy from the field and are directed to move towards higher potential. As a result, the electrons acquire a constant velocity known as *Drift velocity* V_d .

The time ‘ τ ’ is known as the relaxation time and it is defined as the time taken by an electron between two successive collisions. That relaxation time is also called *mean free time* [or] *collision time*.

Electrons are assumed to achieve thermal equilibrium with their surroundings only through collision. These collisions are assumed to maintain local thermodynamic equilibrium in a particularly simple way.

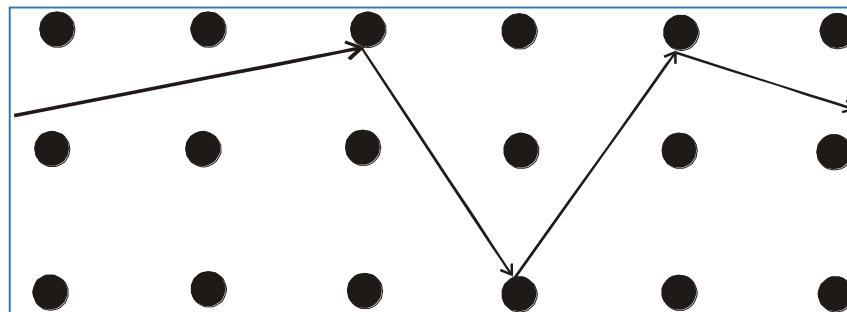


Figure 2 | Trajectory of a conduction electron



Success of classical free electron theory:

- (1). It verifies Ohm's law.
- (2). It explains the electrical and thermal conductivities of metals.
- (3). It derives Wiedemann – Franz law. (i.e., the relation between electrical conductivity and thermal conductivity)
- (4). It explains optical properties of metals.



Drawbacks of classical free electron theory:

1. The phenomena such a photoelectric effect, Compton effect and the black body radiation couldn't be explained by classical free electron theory.
2. Cannot explain the electrical conductivity of semiconductors and Insulators.
3. Ferromagnetism cannot be explained by theory.



QUANTUM FREE ELECTRON THEORY

Classical free electron theory could not explain many physical properties.

In 1928, Sommerfield developed a new theory applying quantum mechanical concepts and Fermi-Dirac statistics to the free electrons in the metal. This theory is called **quantum free electron theory**.

Classical free electron theory permits all electrons to gain energy. But quantum free electron theory permits only a fraction of electrons to gain energy.

According to Quantum mechanics moving particles has some sort of wave motion

Then wavelength $\lambda = h/p$ (De-Broglie wavelength)

To characterize moving particle having wave motion-(ψ)-wavefunction is introduced

According to quantum theory of free electrons energy of a free electron is given by

$$E_n = n^2 h^2 / 8mL^2$$

- According to quantum theory of free electrons the electrical conductivity is given by

$$\sigma = ne^2 T/m$$



MERITS OF QUANTUM FREE ELECTRON THEORY

1. It successfully explains the electrical and thermal conductivity of metals.
2. We can explain the Thermionic phenomenon.
3. Temperature dependence of conductivity of metals can be explained by this theory.
4. It can explain the specific heat of metals.
5. It explains magnetic susceptibility of metals.

DEMERITS OF QUANTUM FREE ELECTRON THEORY

1. It is unable to explain the metallic properties exhibited by only certain crystals
2. Failed to give difference of metals/semiconductors/ insulators
3. It is unable to explain why the atomic arrays in metallic crystals should prefer certain structures only



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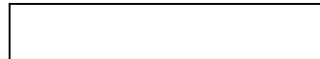
LECTURE 2

**DENSITY OF STATES
ENERGY BANDS IN SOLIDS**



Energy Levels

Empty conduction band



Valence band, filled with electrons



Conduction band, half filled with electrons

$n=3$



$n=2$



$n=1$

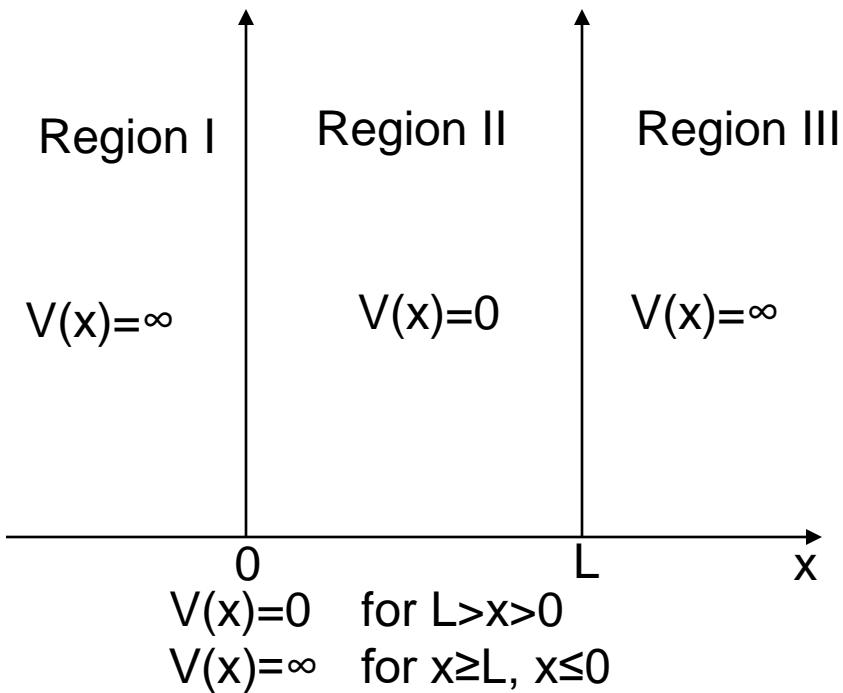


Valence band, filled with electrons



Basics

Particle in a 1-Dimensional Box



Classical Physics: The particle can exist anywhere in the box and follow a path in accordance to Newton's Laws.

Quantum Physics: The particle is expressed by a wave function and there are certain areas more likely to contain the particle within the box.

Time Dependent Schrödinger Equation

$$\frac{-\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + V(x)\Psi = E\Psi$$

$\underbrace{}_{\text{KE}}$ $\underbrace{}_{\text{PE}}$ $\underbrace{}_{\text{TE}}$

Wave function is dependent on time and position function:

$$\Psi(x, t) = f(t)\psi(x)$$

Time Independent Schrödinger Equation

$$\frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi = E\psi$$

Applying boundary conditions:

Region I and III:

$$\frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + \infty^*\psi = E\psi \longrightarrow |\psi|^2 = 0$$

Region II:

$$\frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi$$

Basics

Finding the Wave Function

$$\frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi \longrightarrow -\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2} E\psi$$

This is similar to the general differential equation:

$$-\frac{d^2\psi(x)}{dx^2} = k^2\psi \rightarrow \psi = A\sin kx + B\cos kx$$

So we can start applying boundary conditions:

$$x=0 \quad \psi=0$$

$$0 = A\sin 0k + B\cos 0k \rightarrow 0 = 0 + B*1 \therefore B = 0$$

$$x=L \quad \psi=0$$

$$0 = A\sin kL \quad A \neq 0 \rightarrow kL = n\pi \quad \text{where } n=\mathbb{N}^*$$

Calculating Energy Levels:

$$k^2 = \frac{2mE}{\hbar^2} \longrightarrow E = \frac{k^2\hbar^2}{2m} \longrightarrow E = \frac{k^2h^2}{2m4\pi^2}$$

$$\hbar = \frac{h}{2\pi}$$

$$E = \frac{n^2\pi^2}{L^2} \frac{h^2}{2m4\pi^2} \longrightarrow E = \frac{n^2h^2}{8mL^2}$$

Our new wave function:

$$\psi_H = A \sin \frac{n\pi x}{L} \quad \text{But what is 'A'?}$$

Normalizing wave function:

$$\int_0^L (A \sin kx)^2 dx = 1$$

$$|A|^2 \left[\frac{x}{2} - \frac{\sin 2kx}{4k} \right]_0^L = 1$$

$$|A|^2 \left[\frac{L}{2} - \frac{\sin 2\frac{n\pi}{L}}{4\frac{n\pi}{L}} \right] = 1$$

Since $n=\mathbb{N}^*$

$$|A|^2 \left(\frac{L}{2} \right) = 1 \rightarrow |A| = \sqrt{\frac{2}{L}}$$

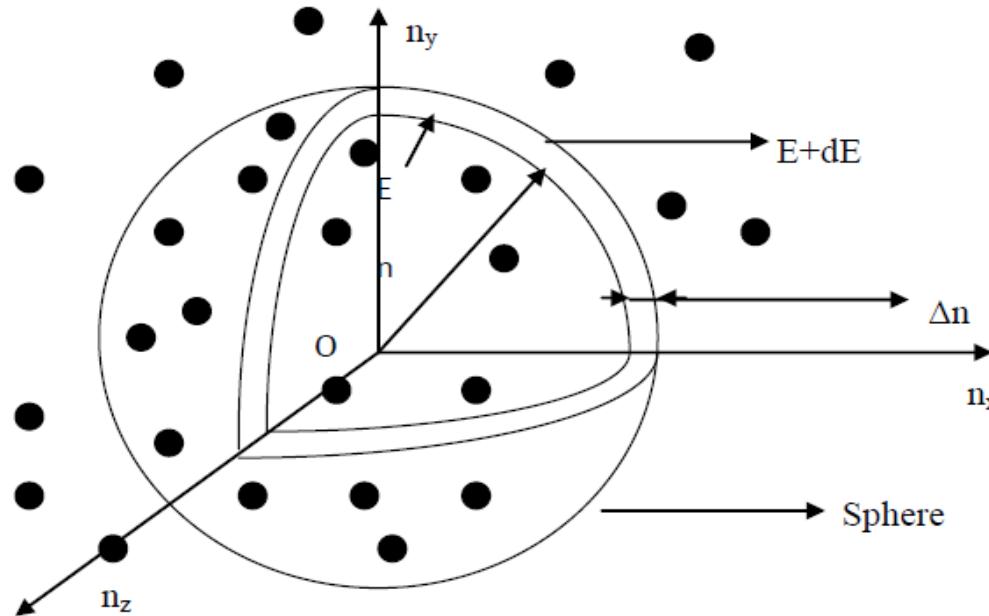
Our normalized wave function

$$\psi_H = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

DENSITY OF STATES



Definition: Density of States $Z(E) dE$ is defined as the number of available electron states per unit volume in an energy interval (dE).



To find the number of energy levels in a cubical metal piece and to find number of electrons that can be filled in a given energy level, let us construct a sphere of radius ' n ' in the space.

DENSITY OF STATES



The sphere is further divided into many shells and each of this shell represents a particular combination of quantum numbers (n_x , n_y , and n_z) and therefore represents a particular energy value.

Let us consider two energy values E and $E + dE$. The number of energy states between E and $E + dE$ can be found by finding the number of energy states between the shells of the radius n and $n + \Delta n$, from the origin.

The number of energy states within the sphere of radius $n = 4/3 \pi n^3$ Since n_x , n_y , and n_z will have only positive values, we have to take only one octant of the sphere (i.e) 1/8 th of the sphere volume.

DENSITY OF STATES

The number of available energy states within the sphere of radius

$$n = 1/8 [4/3 \pi n^3]$$

Similarly the number of available energy states within the sphere of radius

$$n + dn = 1/8 [4/3 \pi (n+dn)^3]$$

The number of available energy states between the shells of radius n and $n + dn$ (or) between the energy levels

$$E \text{ and } E + dE = 1/8 [4/3 \pi (n+dn)^3 - 4/3 \pi n^3]$$

The number of available energy states between the energy interval

$$Z(E)dE = 1/8 \times 4/3 \pi [n^3 + dn^3 + 3n^2dn + 3dn^2n - n^3]$$

DENSITY OF STATES



Since the higher powers of dn is very small, dn^2 and dn^3 terms can be neglected.

$$Z(E)dE = \pi / 6 (3n^2 dn)$$

$$Z(E)dE = \pi / 2(n^2 dn) \quad \longrightarrow \quad (1)$$

We know the energy of the electron in a cubical metal piece of sides ℓ

$$E = -\frac{n^2 h^2}{8m \ell^2}$$

$$n^2 = -\frac{8m \ell^2 E}{h^2} \quad \longrightarrow \quad (2)$$

$$n = \left[\frac{8m \ell^2 E}{h^2} \right]^{1/2} \quad \longrightarrow \quad (3)$$



DENSITY OF STATES

Differentiating equation (2) we get

$$2ndn = \frac{8m \ell^2}{h^2} dE \longrightarrow (4)$$

$$ndn = \frac{8m \ell^2}{2 h^2} dE$$

Equation 1 can be written as

$$Z(E)dE = \pi / 2(n^2 dn)$$

$$Z(E)dE = \pi / 2 n (n dn)$$

Substituting equation (3) and (4) in the above equation we have

$$Z(E)dE = \pi / 2 \left[\frac{8m \ell^2 E}{h^2} \right]^{1/2} \left[\frac{8m \ell^2}{2 h^2} dE \right]$$

DENSITY OF STATES



$$Z(E)dE = \pi / 4 \left[\frac{8m \ell^2}{h^2} \right]^{3/2} E^{1/2} dE$$

$$Z(E)dE = \pi / 4 \left[\frac{8m}{h^2} \right]^{3/2} \ell^3 \cdot E^{1/2} dE$$

Here ℓ^3 represents the volume of the metal piece. If $\ell^3 = 1$, then we can write that

The number of available energy states per unit volume (i.e) Density of states

DENSITY OF STATES



$$Z(E)dE = \pi / 4 \left[\frac{8m}{h^2} \right]^{3/2} E^{1/2} dE \longrightarrow (5)$$

Since each energy level provides 2 electron states one with spin up and another spin down, we have

Density of states

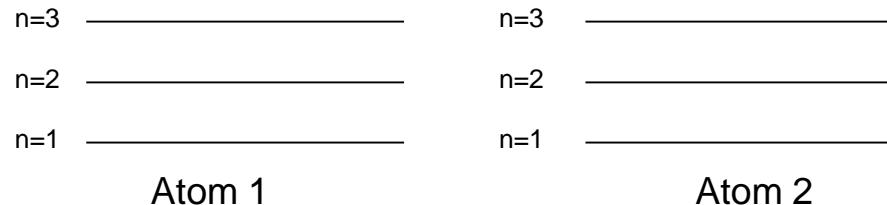
$$Z(E)dE = 2 \times \pi / 4 \left[\frac{8m}{h^2} \right]^{3/2} E^{1/2} dE$$

$$Z(E)dE = \pi / 2 \left[\frac{8m}{h^2} \right]^{3/2} E^{1/2} dE \longrightarrow (6)$$

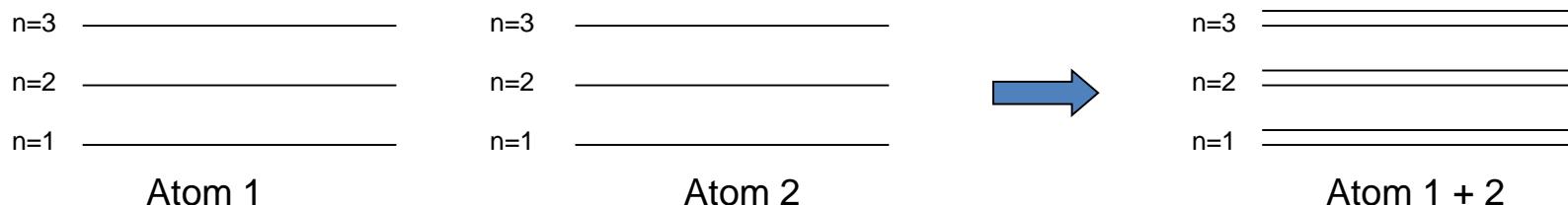


Energy bands in solids

- A solid is formed by bringing together isolated single atoms.
- Consider the combination of two atoms. If the atoms are far apart there is no interaction between them and the energy levels are the same for each atom. The numbers of levels at a particular energy is simply doubled



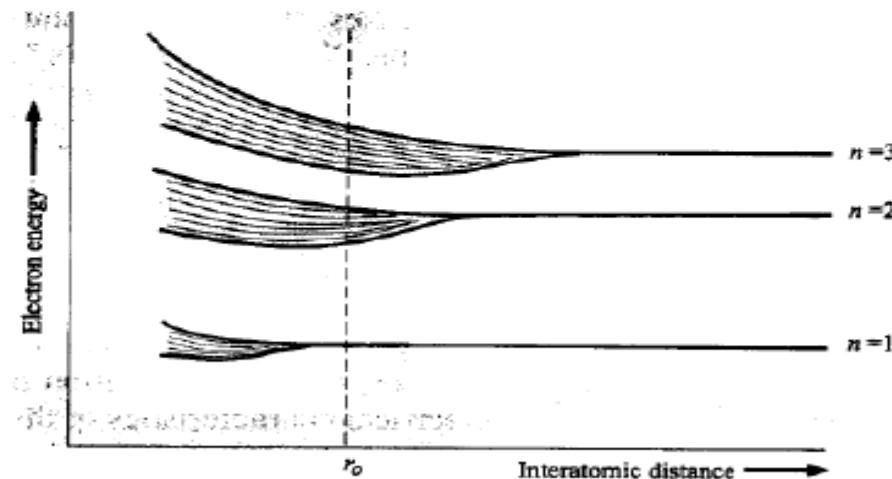
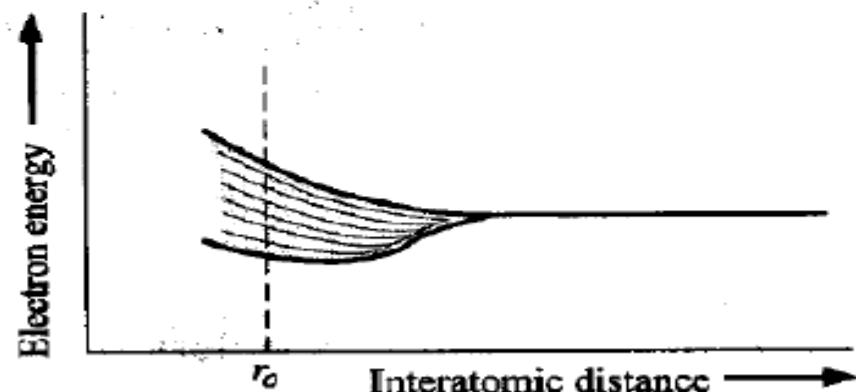
- If the atoms are close together the electron wave functions will overlap and the energy levels are shifted with respect to each other.



Energy bands in solids



- Consider a regular periodic arrangement of atoms in which each atom contains more than one electron. If the atoms are initially far apart, the electrons in adjacent atoms will not interact and will occupy the discrete energy levels.
- If the atoms are brought closer enough, the outmost electrons will interact and the energy levels will split into a band of allowed energies.



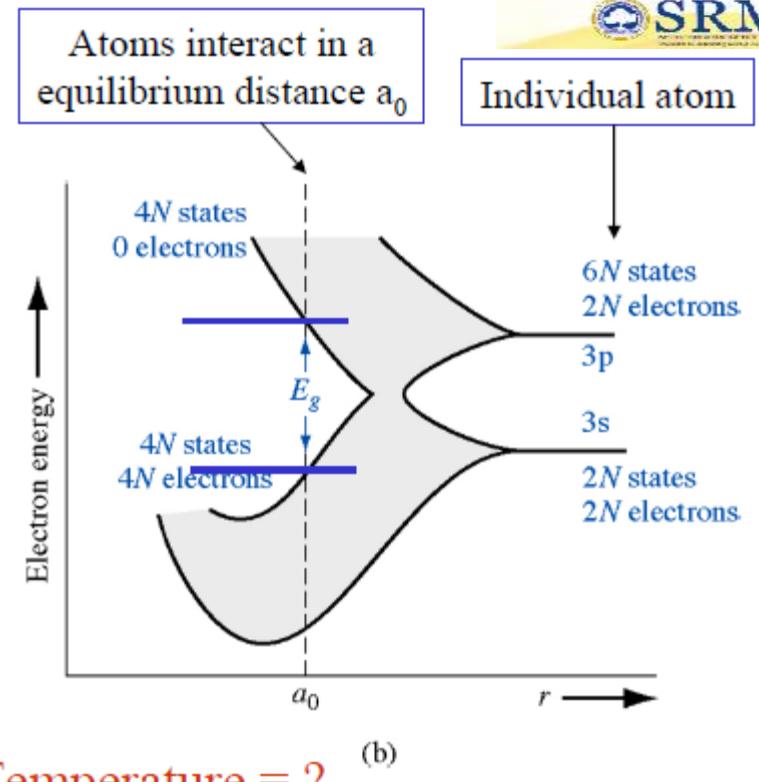
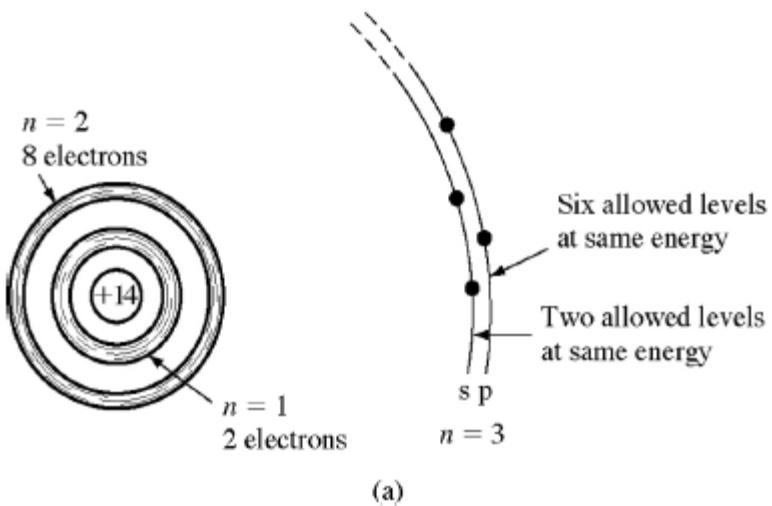
The splitting of an energy state into a band of allowed energies.



Energy bands in solids



$1s^2 2s^2 2p^6 3s^2 3p^{2+4}$



- (a) Schematic of an isolated Si atom. (b) The splitting of the $3s$ and $3p$ states of silicon into allowed and forbidden energy bands.



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Lecture 3

KRONIG PENNEY MODEL

According to quantum free electron theory of metals, *a conduction electron in a metal experiences constant (or zero) potential and free to move inside the crystal* but will not come out of the metal because an infinite potential exists at the surface.

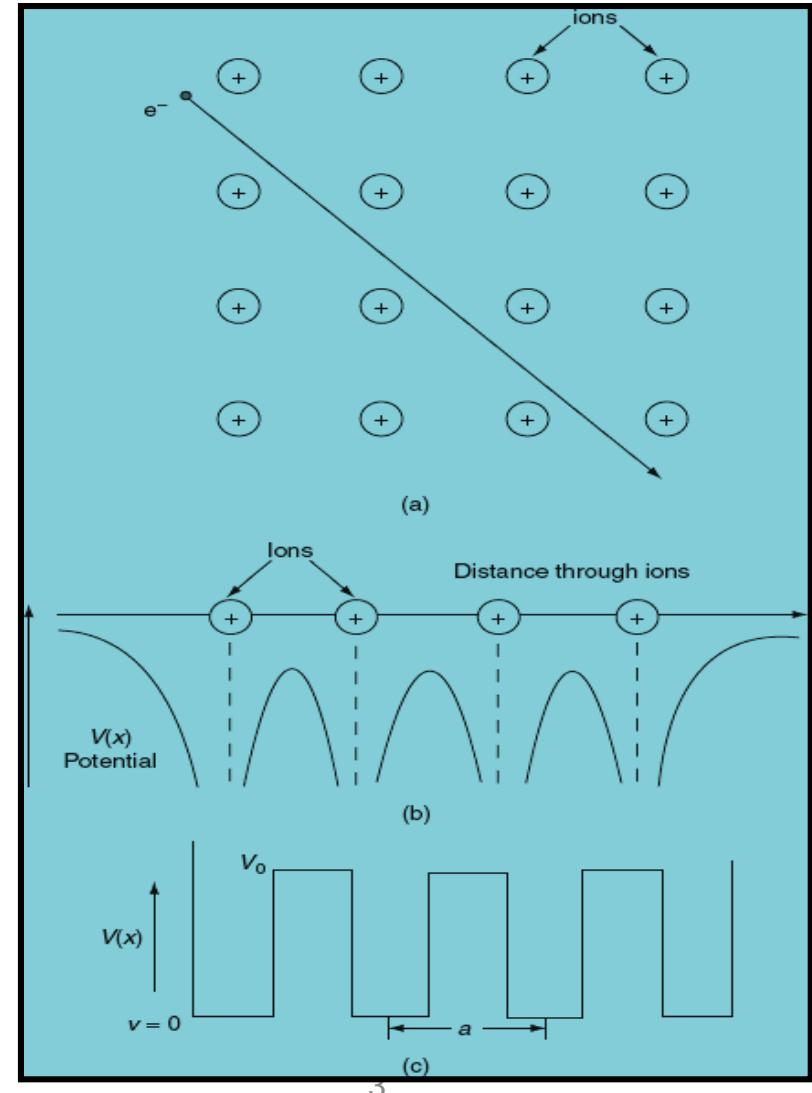
This theory successfully explains electrical conductivity, specific heat, thermionic emission and paramagnetism.

This theory fails to explain many other physical properties, for example it fails to explain

- (i) the difference between conductors, insulators and semiconductors
- (ii) positive Hall coefficient of metals and
- (iii) lower conductivity of divalent metals than monovalent metals.

To *overcome the above problems, the periodic potentials due to the positive ions in a metal* have been considered shown in Fig. (a), if an electron moves through these ions, it experiences varying potentials.

The potential of an electron at the positive ion site is zero and is maximum in between two ions. The potential experienced by an electron, when it passes along a line through the positive ions is as shown in Fig. (b).



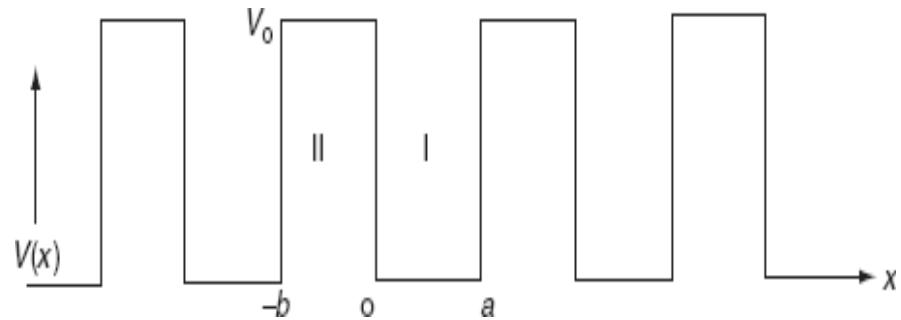
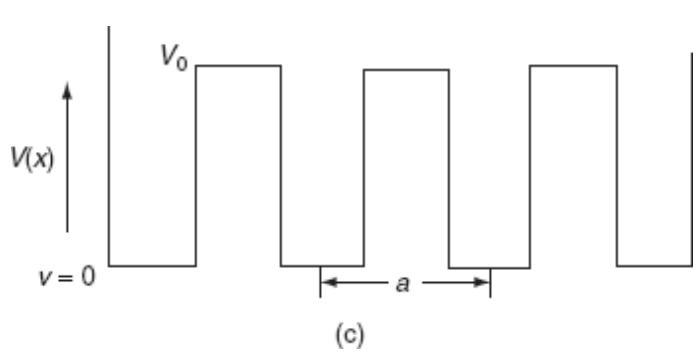
Kronig Penney model for 1 D Periodic Potential:

- According to Kronig and Penney the electrons move in a periodic square well potential.
- This potential is produced by the positive ions (ionized atoms) in the lattice.
- The potential is zero near to the nucleus of positive ions and maximum between the adjacent nuclei. The variation of potential is shown in figure.

Kronig Penney Model



It is not easy to solve Schrödinger's equation with these potentials. So, Kronig and Penney approximated these potentials inside the crystal to the shape of rectangular steps as shown in Fig. (c). This model is called Kronig-Penney model of potentials.



The energies of electrons can be known by solving Schrödinger's wave equation in such a lattice.

The energies and wave functions of electrons associated with this model can be calculated by solving time-independent one-dimensional Schrödinger's wave equations for the two regions I and II as shown in Figure.



Kronig Penney Model



The Schrodinger equations for two regions are

and $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \psi = 0 \quad \text{for } -b < x < 0 \quad \dots\dots\dots 2$

If $V_0 > E$ and α, β are real quantities then equations 1 and 2 will become



Kronig Penney Model



where

The potential is periodic *i.e.*,

$$V(x) = V(x + a + b) \quad \dots \dots \dots 6$$

According to Bloch, the Solutions of the Schrodinger equations are of the form

where $u_k(x)$ is a periodic function with the periodicity of lattice i.e.,



Kronig Penney Model



Therefore, equations 3 and 4 can be written as

The solutions of these equations 9 and 10 are,

where A, B, C and D are constants

Kronig Penney Model



$$\frac{d\Psi}{dx} = e^{ikx} \frac{du_K}{dx} + u_K iK e^{ikx}$$

and $\frac{d^2\Psi}{dx^2} = e^{ikx} \frac{d^2u_K}{dx^2} + iK e^{ikx} \frac{du_K}{dx} + iK e^{ikx} \frac{du_K}{dx} - K^2 e^{ikx} u_K$

i.e., $\frac{d^2\Psi}{dx^2} = -K^2 e^{ikx} u_K + 2iK e^{ikx} \frac{du_K}{dx} + e^{ikx} \frac{d^2u_K}{dx^2}$

Kronig Penney Model



These constants can be determined in such a way that the wave function Ψ and its derivative $d\Psi/dx$ are single valued and continuous

i.e.,

$$u_1(0) = u_2(0), \quad u_1(a) = u_2(-b)$$

$$\frac{du_1}{dx} \Big|_{x=0} = \frac{du_2}{dx} \Big|_{x=0}$$

$$\frac{du_1}{dx} \Big|_{x=a} = \frac{du_2}{dx} \Big|_{x=-b}$$

..... 13

Using these boundary conditions, we get

$$A + B = C + D$$

$$Ai(\alpha - k) - Bi(\alpha + k) = C(b - ik) - D(\beta + ik)$$

$$Ae^{i(\alpha - k)} + Be^{-i(\alpha + k)a} = Ce^{-(\beta - ik)\beta} + De^{(\beta + ik)\beta}$$

$$\text{and } Ai(\alpha - k)e^{i(\alpha - k)a} - Bi(\alpha + k)e^{-i(\alpha + k)a}$$

$$= C(\beta - ik)e^{-(\beta - ik)b} - D(\beta + ik)e^{(\beta + ik)b} \quad 14$$

Kronig Penney Model



These equations have non-zero solutions if the determinant of the coefficients A, B, C and D vanishes. That is

$$\begin{vmatrix} 1 & 1 & 1 & 1 \\ i(\alpha - k) & -i(\alpha + k) & (\beta - ik) & -(\beta + ik) \\ e^{i(\alpha - k)a} & e^{-i(\alpha + k)a} & e^{(\beta i - k)b} & e^{(\beta i + k)b} \\ i(\alpha - k)e^{i(\alpha - k)a} & -i(\alpha + k)e^{-i(\alpha + k)a} & (\beta - ik)e^{-(\beta - ik)b} & -(\beta + ik)e^{(\beta + ik)b} \end{vmatrix} = 0 \quad 15$$

On expanding this determinant and after simplification, we get

$$P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka \quad 16$$

Where the quantity P is defined as

$$P = \frac{\beta^2 ab}{2} = \frac{2mv_0 ab}{2h^2} = \frac{mv_0 ab}{h^2} \quad 17$$

Kronig Penney Model



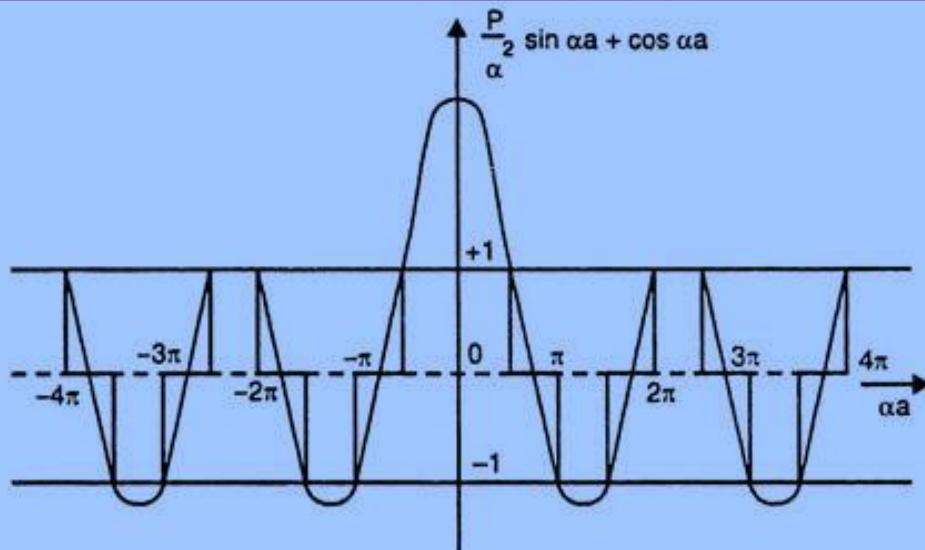
$$P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

This equation shows the relation between the energy (through α) and the wave-vector, k , and as you can see, since the left hand side of the equation can only range from -1 to 1 then there are some limits on the values that α (and thus, the energy) can take, that is, at some ranges of values of the energy, there is no solution according to these equation, and thus, the system will not have those energies: *energy gaps*. These are the so-called band-gaps, which can be shown to exist in *any* shape of periodic potential (not just delta or square barriers).

Kronig Penney Model



If we plot a graph between $\cos ka$ and αa for P , we get the curve as shown in Fig. Since $\alpha = \sqrt{2mE/h^2}$, the abscissa αa is a measure of energy and by finding the value of αa at any point, the energy represented by the function at that point is calculated. The values of αa satisfying final equation are obtained by drawing a line parallel to αa -axis at a distance $\cos ka$ from it. If we change αa continuously from 0 to i.e., $\cos ka = \pm 1$, we obtain all possible values of αa and hence that of energy



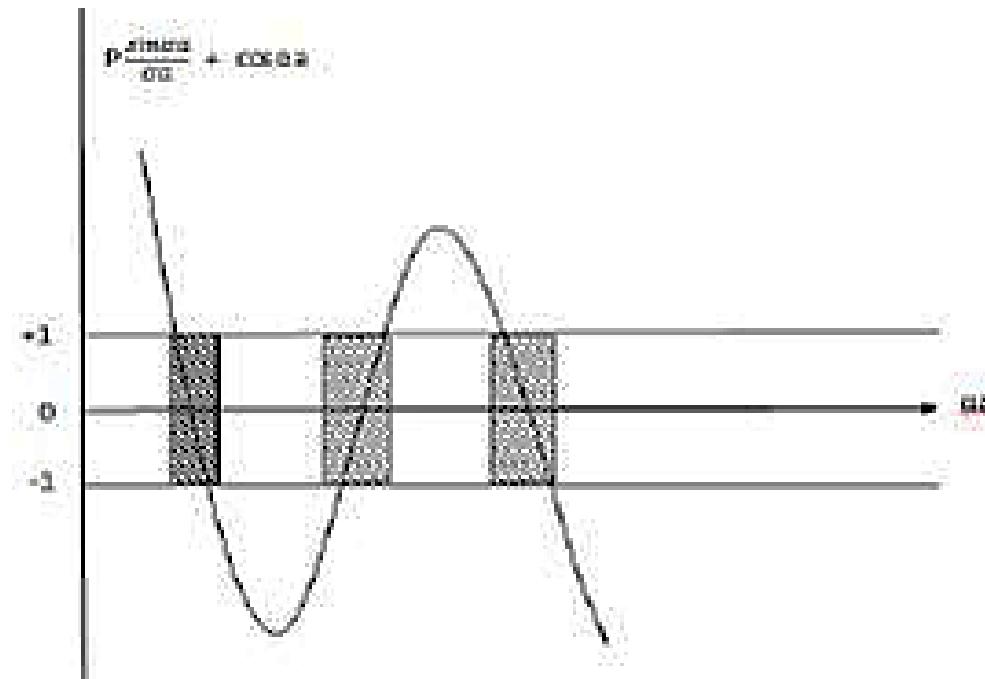
Plot of $(P/\alpha a) \sin \alpha a + \cos \alpha a$ as a function of αa using $P = (3\pi/2)$. The solid and broken lines on the abscissa correspond to allowed and forbidden energy regions respectively.



Kronig Penney Model

Special Cases:

Case 1: The permissible limit of the term $P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$ lies between +1 to -1. By varying αa , a wave mechanical nature could be plotted as shown in Fig, the shaded portion of the wave shows the bands of allowed energy with the forbidden region as unshaded portion.





Kronig Penney Model



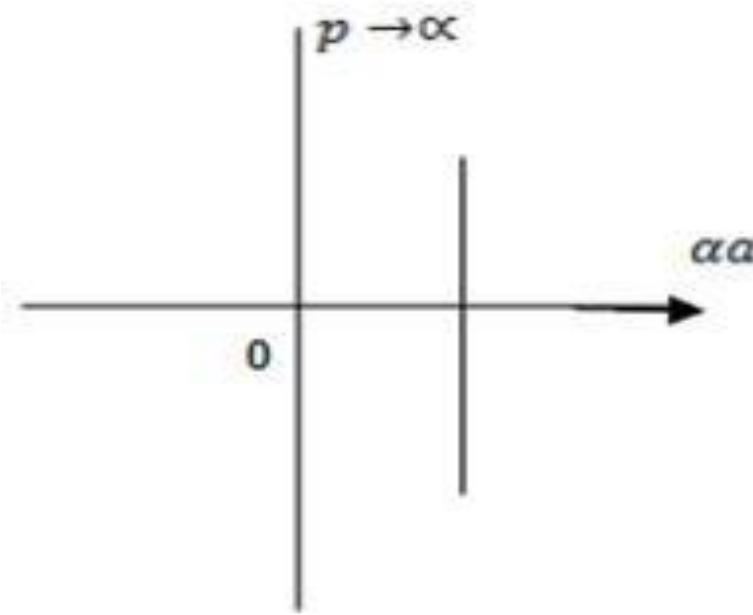
Special Cases:

With increase of αa , the allowed energy states for a electron increases thereby increasing the band width of the bands, i.e., the strength of the potential barrier diminishes. This also leads to increase of the distance between electrons and the total energy possessed by the individual electron.

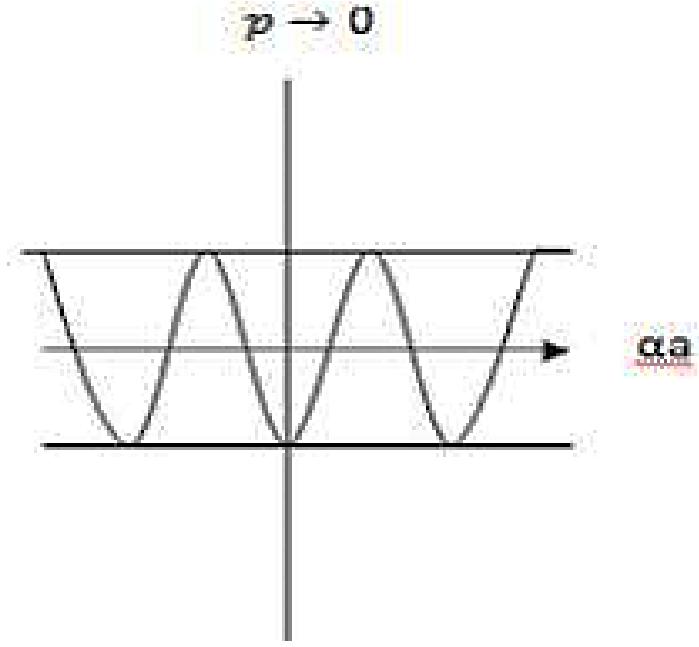
Case 2: Conversely if suppose the effect of potential barrier dominate i.e., if P is large, the resultant wave obtained in terms of shows a stepper variation in the region lies between +1 to -1. This results in the decrease of allowed energy and increase of forbidden energy gap. Thus at extremities,



Kronig Penney Model



(a) When $P \rightarrow \alpha$, the allowed energy states are compressed to a line spectrum



(b) When $P \rightarrow 0$, when the energy band is broadened and it is quasi continuous.



DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

18PYB103J –Semiconductor Physics

Lecture-4

SOLVING PROBLEMS



1. The electrical resistivity of copper at 27°C is $1.72 \times 10^{-8} \text{ Ohm m}$. Compute its thermal conductivity if the Lorentz number is $2.26 \times 10^{-8} \text{ W Ohm K}^{-2}$

Given (ρ) = $1.72 \times 10^{-8} \text{ Ohm m}$

$T = 27^\circ \text{C} \Rightarrow 273 + 27 = 300 \text{ K}$

$L = 2.26 \times 10^{-8} \text{ W Ohm K}^{-2}$

According to Wiedemann - Franz law using classical free electron theory

$$\frac{k}{\sigma} = LT$$

(or) $k = \sigma LT$

$$k = \frac{LT}{\rho} \quad [\because \sigma = \frac{1}{\rho}]$$

Therefore thermal Conductivity $k = \frac{2.26 \times 10^{-8} \times 300}{1.72 \times 10^{-8}}$

$$k = 394.18 \text{ W m}^{-1} \text{ K}^{-1}$$

2. Calculate the drift velocity of electrons in copper and current density in wire of diameter 0.16 cm which carries a steady current of 10 A. Given $n = 8.46 \times 10^{28} \text{ m}^{-3}$.

Solution:

Given:

$$\begin{aligned}\text{Diameter of the wire } d &= 0.16 \text{ cm} \\ \text{Current flowing} &= 10 \text{ A}\end{aligned}$$

$$\begin{aligned}\text{Current density } J &= \frac{\text{Current}}{\text{Area of cross section (A}^2\text{)}} \\ &= \frac{10}{\pi r^2} = \frac{10}{\pi(d/2)^2} \quad \left[\because r = \frac{d}{2} \right] \\ &= \frac{10}{3.14 \times [0.16 \times 10^{-2}/2]^2} \\ J &= 4.976 \times 10^6 \text{ Am}^{-2} \\ J &= neV_d \\ V_d &= \frac{J}{ne} \\ &= \frac{4.97 \times 10^6}{8.46 \times 10^{28} \times 1.6 \times 10^{-19}} \\ \text{Drift velocity } V_d &= 3.67 \times 10^{-4} \text{ m s}^{-1}\end{aligned}$$



3. Find the lowest energy of an electron confined in one dimensional potential box separated by distance 0.1 nm.

Given $l = 0.1 \text{ nm} \Rightarrow$ we know $\hbar = 6.62 \times 10^{-34}$

We know Energy of electron in 1-D Box is

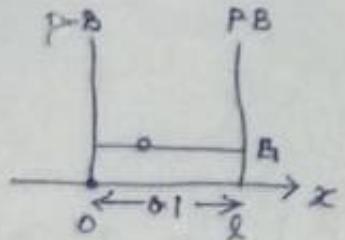
$$E_n = \frac{n^2 \hbar^2}{8ml^2}$$

To find, Lowest energy of an electron ($n=1$)

$$E_1 = \frac{(1)^2 \times (6.62 \times 10^{-34})^2}{8 \times (9.1 \times 10^{-31}) \times (0.1 \times 10^{-9})^2}$$

$$E_1 = \frac{4.38244 \times 10^{-67}}{7.28 \times 10^{-31} \times 10^{-18}} = \frac{4.38244 \times 10^{67}}{7.28 \times 10^{-49}}$$

$$E_1 = 6.0198 \times 10^{-19} \text{ J}$$





4. An electron is bound in one dimensional infinite well of width 1×10^{-10} m. Find the energy value in the ground state, first and second excited states.

we know $E_n = \frac{\hbar^2 h^2}{8m\ell^2}$

To find lowest energy of an electron ($n=1$)

$$E_1 = \frac{(1)^2 \times (6.62 \times 10^{-34})^2}{8 \times (9.1 \times 10^{-31}) \times (1 \times 10^{-10})^2}$$

$$E_1 = 0.6031 \times 10^{-17} \text{ J}$$

$$\begin{aligned}\text{Energy of first excited state} &= 4 \times 0.6031 \times 10^{-17} \\ &= 2.412 \times 10^{-17} \text{ J}\end{aligned}$$

$$\begin{aligned}\text{Energy of second excited state} &= 9 \times 0.6031 \times 10^{-17} \\ &= 5.428 \times 10^{-17} \text{ J}\end{aligned}$$



5. Find the least energy of an electron moving in one-dimensional potential box (infinite height) of width 0.05nm.

$$E_n = \frac{n^2 h^2}{8mL^2} \quad L = 0.05 \text{ nm} = 0.05 \times 10^{-9} \text{ m}$$

$$E_1 = \frac{h^2}{8mL^2} = \frac{(6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times 0.5 \times 10^{-10} \times 0.5 \times 10^{-10}} \text{ J}$$

$$= \frac{6.63 \times 6.63}{8 \times 9.1 \times 0.25} \times 10^{-17} \text{ J} = 2.4 \times 10^{-17} \text{ J}$$

$$= \frac{2.4 \times 10^{-17}}{1.6 \times 10^{-19}} = 150.95 \text{ eV}$$



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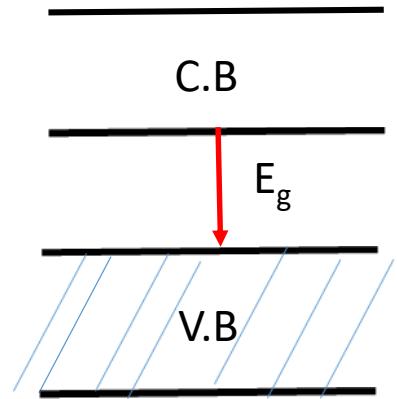
18PYB103J –Semiconductor Physics

Lecture 7

**E-K DIAGRAM
&
DIRECT AND INDIRECT BANDGAP SEMICONDUCTORS**

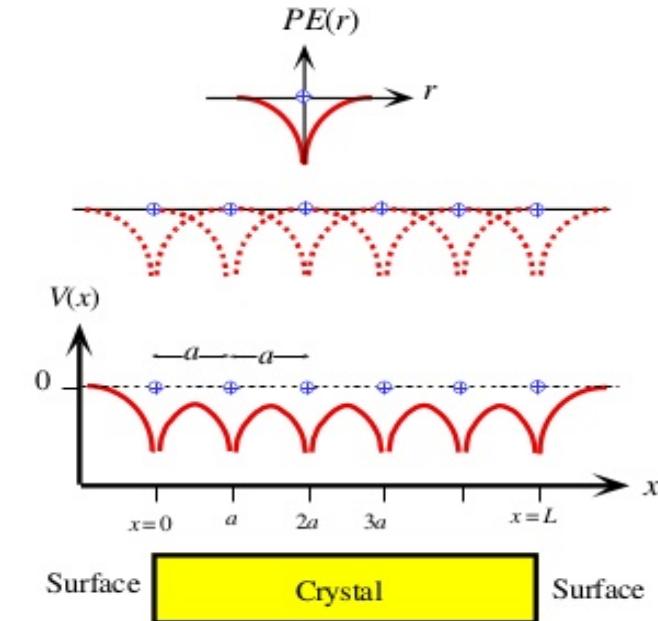
E-K Diagram

- The conventional band diagram shows the band gap energy only
- To know more electrical and optical properties of semiconductor material we need to know E-K diagram
- An E-K diagram shows characteristics of particular semiconductor material
- It shows the relationship between energy and momentum of available states for electron in the crystal
- K being the momentum and E as the energy from a mathematical point of view K is the wave vector
- The E-K diagram of semiconductor is obtained by solving the Schrodinger's equation.



Bloch Theorem

- Most of the semiconductors are in crystalline form, i.e the atoms are arranged in periodic manner.
- The motion of electron in a crystal is governed by the laws of quantum mechanics.
- If we have one electron and one proton system like hydrogen atom it is easy to solve Schrodinger equation.
- But in solid there are large number of atoms and electrons present, so its very difficult to solve the Schrodinger equation.
- If we consider a one dimensional periodic lattice and the potential energy (PE) of a moving electron depends on its position inside the lattice, but the PE is said to be periodic in nature by F. Bloch, and the probability of finding a electron is also periodic, the wave-function associated with electron is also periodic in nature.
- Since the probability of finding electron is equal to $|\Psi|^2$



PE of the electron around an isolated atom

When N atoms are arranged to form the crystal then there is an overlap of individual electron PE functions.

PE of the electron, $V(x)$, inside the crystal is periodic with a period a .

The electron potential energy (PE), $V(x)$, inside the crystal is periodic with the same periodicity as that of the crystal, a . Far away outside the crystal, by choice, $V = 0$ (the electron is free and $PE = 0$).

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Schrödinger's one-Dimensional time independent wave equation

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2} (E - V)\Psi = 0 \quad \text{---(1)}$$

Bloch postulated that the potential (V) inside the crystal is periodic, so V can be written as $V(x)$ for one dimensional lattice.

Again the periodic potential $V(x)$ can be written as by means of lattice constant $V(x+a)$

$$\text{i.e } V(x) = V(x+a) \quad \text{---(2)}$$

Bloch also postulated that the wave function of an electron moving in a periodic lattice is periodic and which is given as

$$\psi_k(x) = e^{ikx} u_k(x) \quad \text{---(3), where } u_k(x) = u_k(x+a) \text{ (periodicity of crystal)}$$

If we substitute the eqs 2 & 3 in eq 1 one can get the solution for the Schrödinger's time independent equation by Numerical and analytical methods

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi_k(x) = 0$$

From the above equation if we plot energy Eigen values vs wave vector K will give the E-K diagram
So the energy Eigen values are periodic in k space

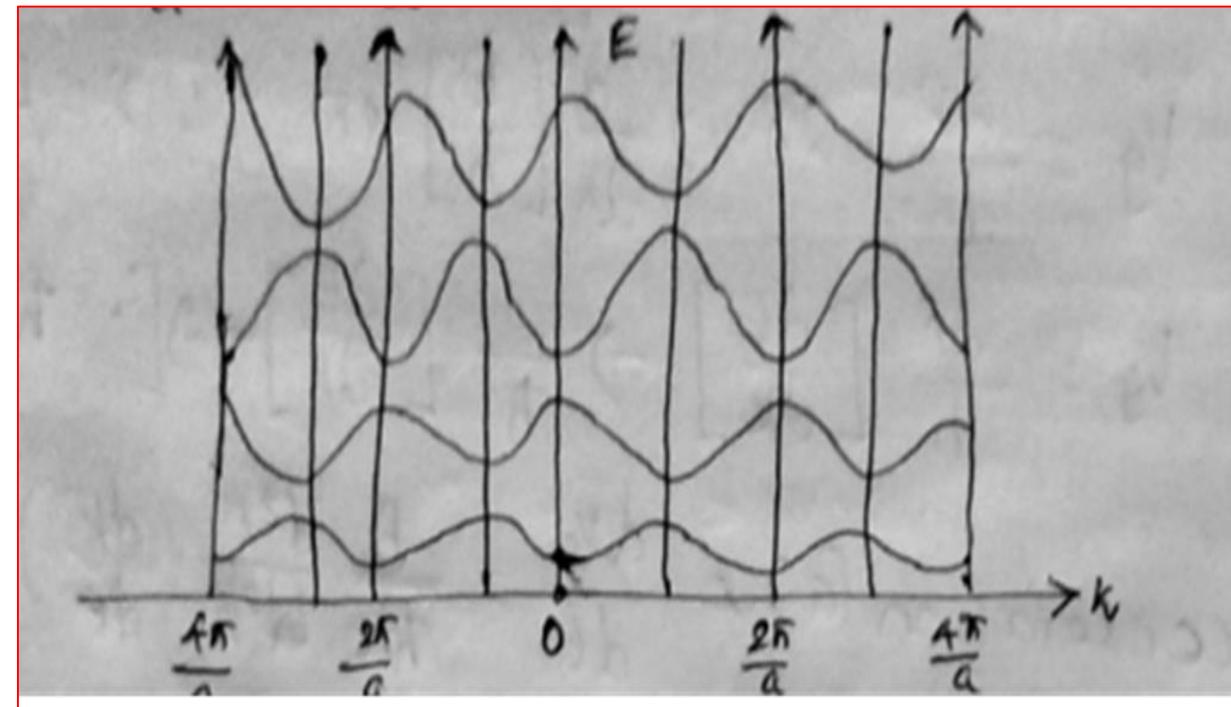


There are three types of E-K diagram

- Periodic zone
- Extended zone
- Reduced zone

Periodic zone scheme:

The periodic repetition of allowed energy values corresponding to each allowed band, which is obtained by the periodic repetition of the region of $-\frac{\pi}{a} < k < \frac{\pi}{a}$ through whole k-space.





Extended Zone Scheme:

In this scheme, different bands are drawn in different zones. In k - space.

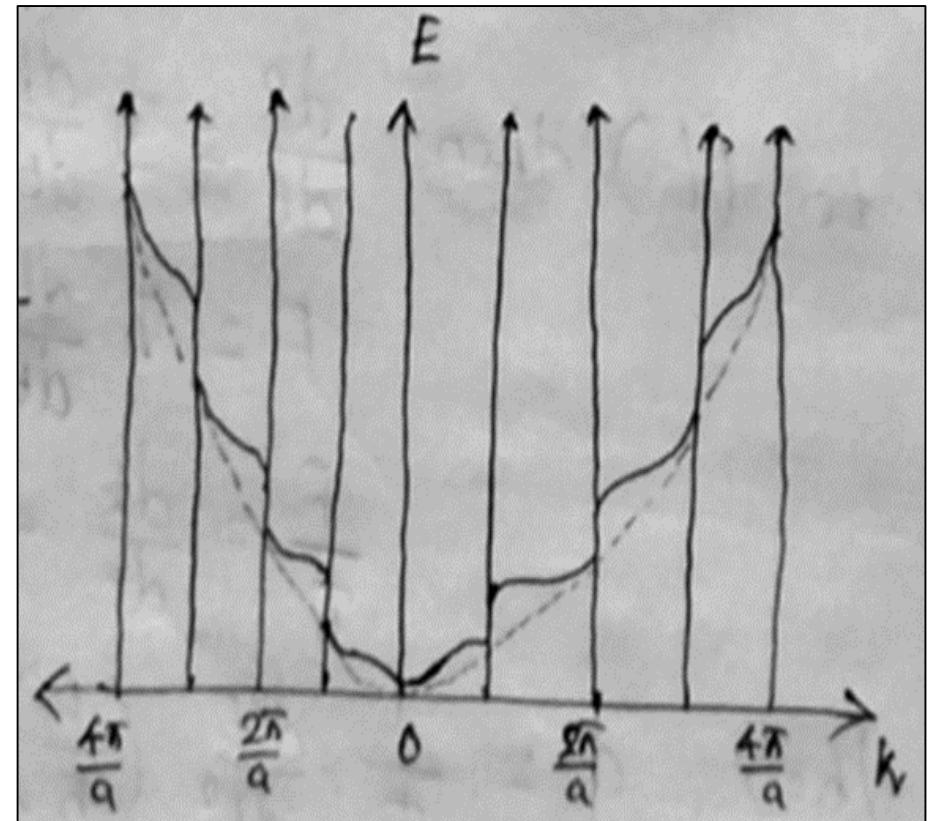
A discontinuities is obtained at $K = \pm \frac{n\pi}{a}$ where $n = \pm 1, \pm 2, \dots$

For $k = -\frac{\pi}{a}$ to $\frac{\pi}{a}$ is first Brillouin zone

For $k = -\frac{\pi}{a}$ to $-\frac{2\pi}{a}$ and $\frac{\pi}{a}$ to $\frac{2\pi}{a}$ is second Brillouin zone

The discontinuities in the curve is due to Braggs law of reflection

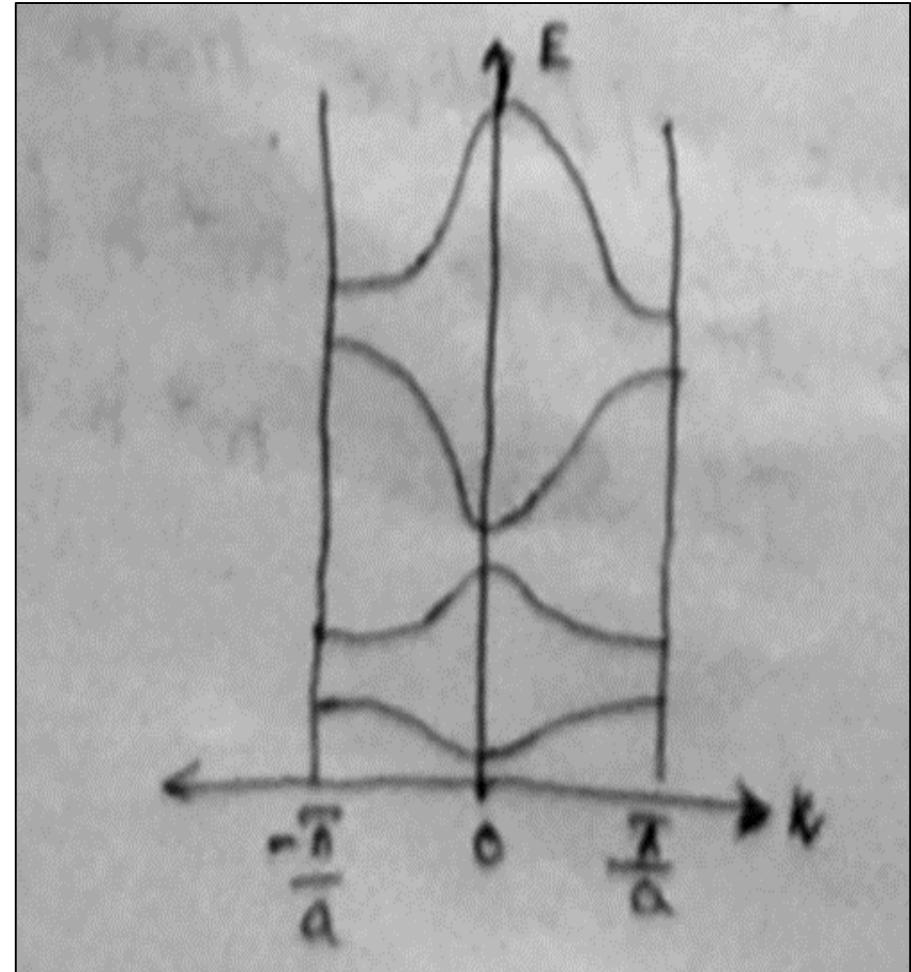
at the edges of allowed bands (i.e) $K = \pm \frac{n\pi}{a}$

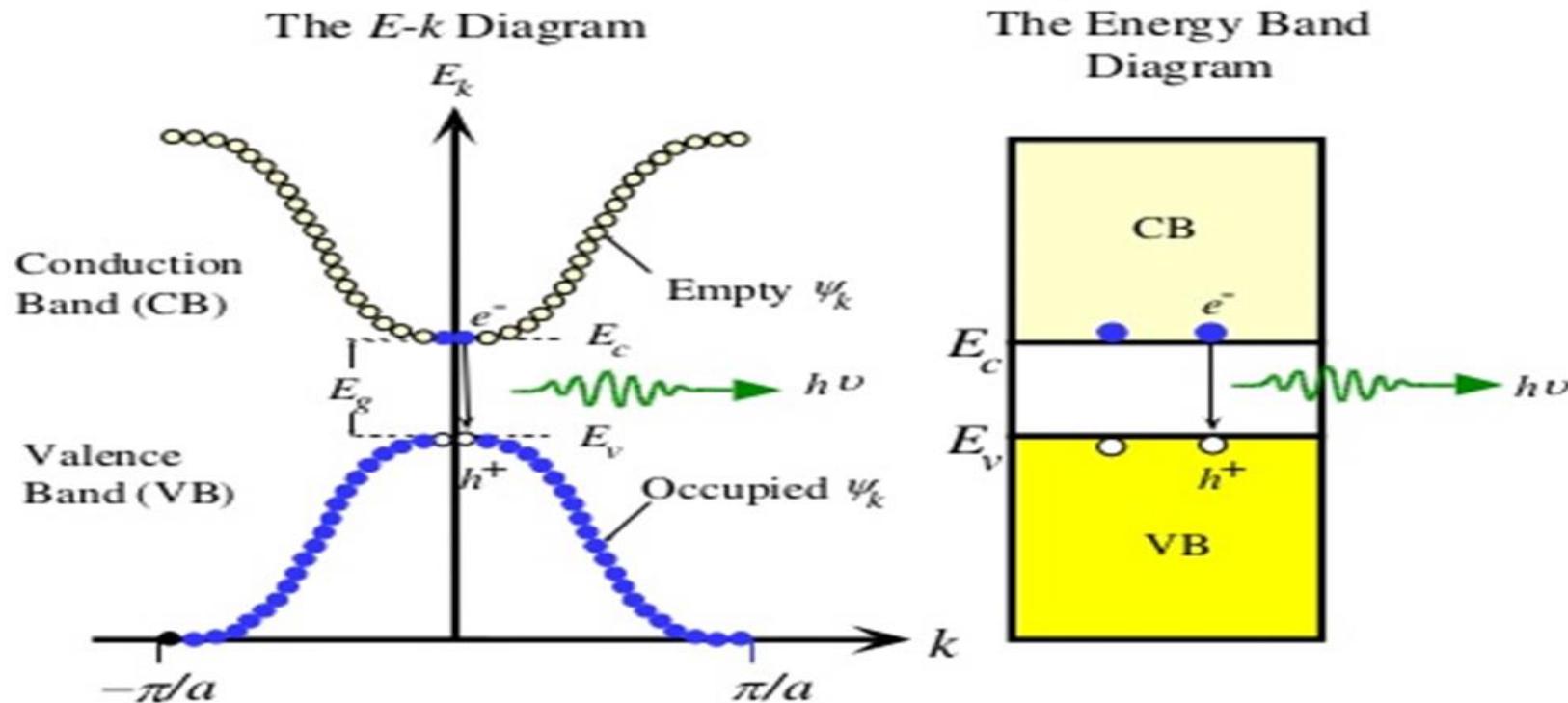




Reduced zone scheme :

- In this scheme the first Brillouin zone is shown since the E-K diagram is periodic, it is sufficient to restrict to first zone in the reduced scheme.
- If we know the energy values of first zone with respect to K then we know every where because energy Eigen values are periodic
- In many of optoelectronic text books the reduce zone scheme is shown





The $E-k$ diagram of a direct bandgap semiconductor such as GaAs. The $E-k$ curve consists of many discrete points with each point corresponding to a possible state, wavefunction $\psi_k(x)$, that is allowed to exist in the crystal. The points are so close that we normally draw the $E-k$ relationship as a continuous curve. In the energy range E_v to E_c there are no points ($\psi_k(x)$ solutions).

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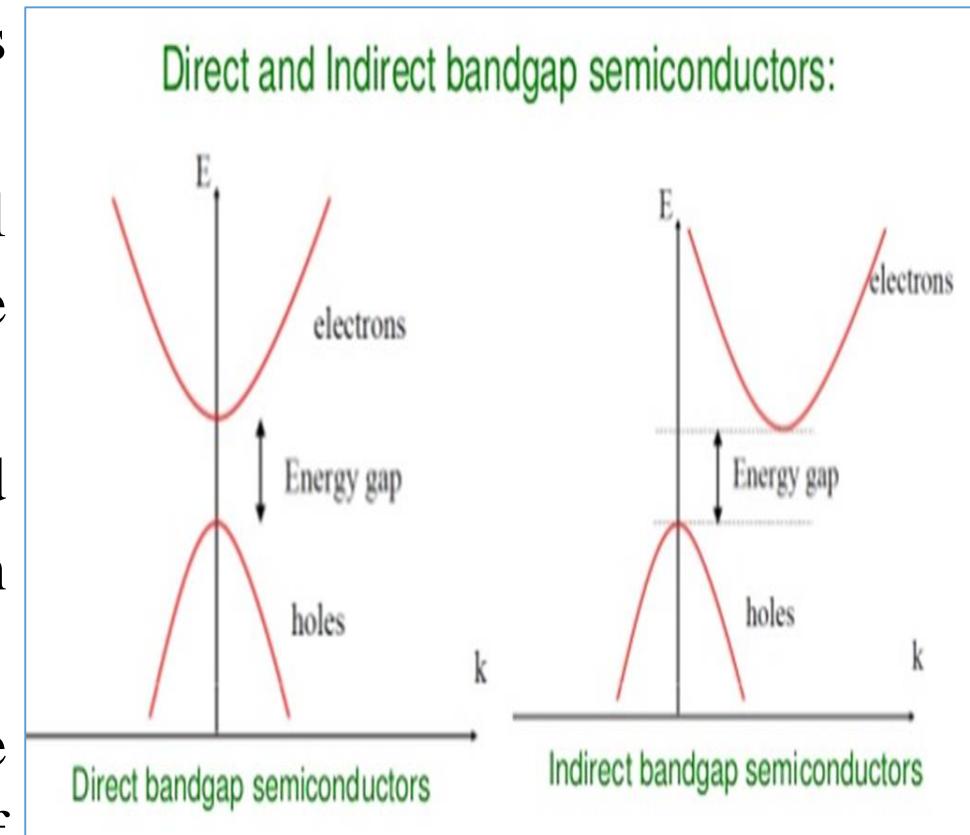
What are the significance of E-K diagram

- No theoretical study, experimentation and technological application can take place without E-K diagram.
- This diagram indicates the band gap E_g which is the difference in energy between top of the valance band and bottom of the conduction band
- This diagram demonstrate electron (hole) mobility
- This diagram explains electron (hole) effective mass
- This diagram indicate how the electron states are equally spaced in K-Space
- This diagram clearly shows direct vs indirect band gap

Direct and Indirect band gap semiconductors



- We know the relation between energy and wave number for an one dimensional lattice. In real crystals the $E - k$ relationship is much more complicated.
- In crystals the interatomic distances and internal potential energy distribution vary with direction of the crystal.
- Hence the $E - K$ relationship and energy band formation depends on the orientation of the electron wave vector to the crystallographic axes.
- In few crystals like GaAs, the maximum of the valence band occurs at the same value of K as the minimum of the conduction band.
- This is called *direct band gap semiconductor*.





Direct and Indirect band gap semiconductors

- In few semiconductors like Si the maximum of the valence band does not always occur at the same K values the maximum of the conduction band. This we call *indirect band gap semiconductor*.
- In direct band gap semiconductors the direction of motion of an electron during a transition across the energy gap, remains unchanged.
- Hence the efficiency of transition of charge carriers across the band gap is more in direct band gap than in indirect band gap semiconductors.



We know

$$P = \hbar k$$

Kinetic energy (K) = $\frac{1}{2}mv^2$, and

Momentum (p) = mv

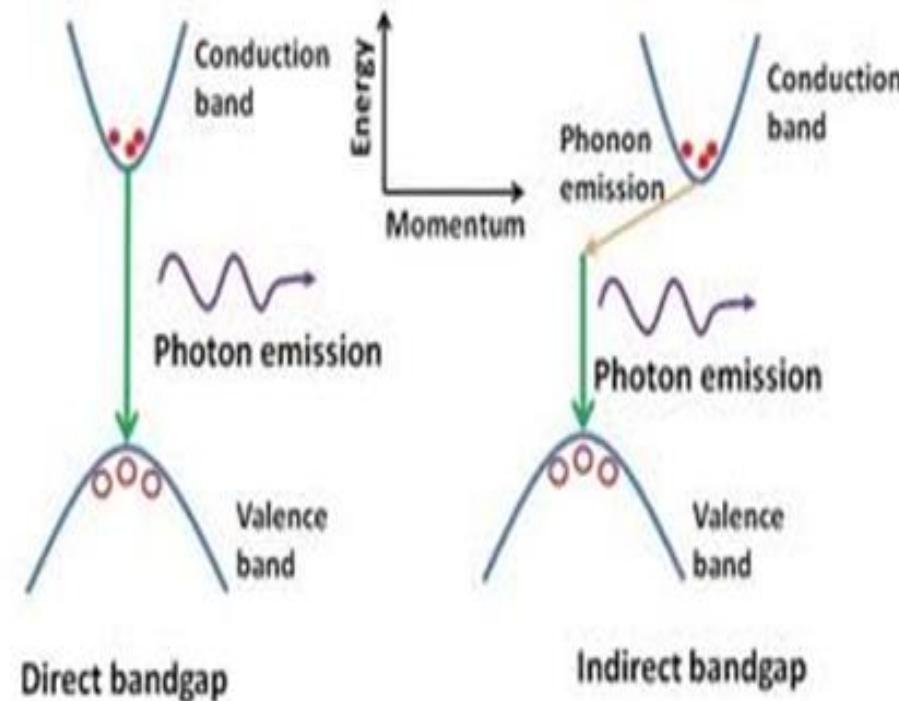
Where, symbols have usual meaning.

Now,

$$K = \frac{1}{2}mv^2 = \frac{1}{2}mv^2 \times \frac{m}{m} = \frac{1}{2} \frac{m^2v^2}{m} = \frac{(mv)^2}{2m} = \frac{p^2}{m}$$

therefore,

$$K = \frac{p^2}{2m}$$

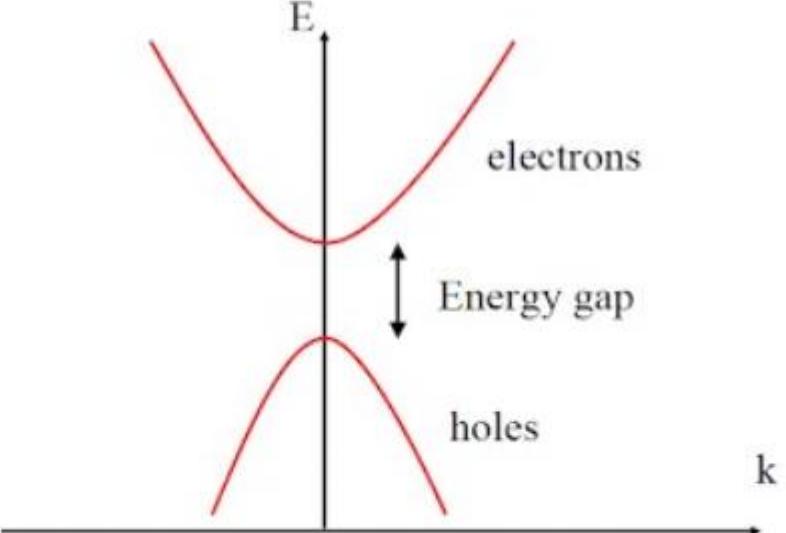
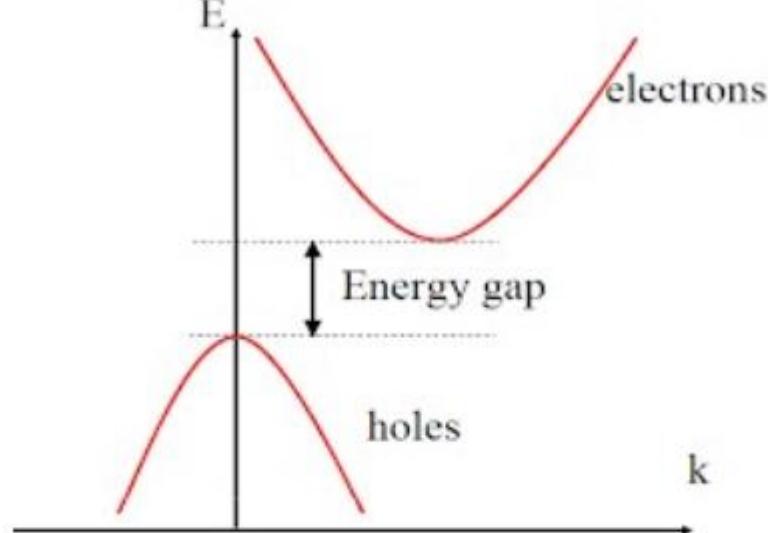


A direct recombination occurs with the release of energy equals to energy difference between two levels such as E_g . The probability of radiative recombination is high and hence direct bandgap semiconductors are used in optical sources

Due to relative difference in momentum, first the momentum is conserved by release of energy only after both the Momentum align themselves. The probability of radiative recombination is comparatively low.



No	Direct Band gap semiconductor	Indirect band gap semiconductor
1	A direct band-gap (DBG) semiconductor is one in which the maximum energy level of the valence band aligns with the minimum energy level of the conduction band with respect to momentum.	A indirect band-gap (DBG) semiconductor is one in which the maximum energy level of the valence band are misaligned with the minimum energy level of the conduction band with respect to momentum.
2	In a DBG semiconductor, a direct recombination takes place with the release of the energy equal to the energy difference between the recombining particles.	Due to a relative difference in the momentum, first, momenta align themselves, a recombination occurs accompanied with the release of energy.
3	The efficiency factor of a DBG semiconductor is higher.	The efficiency factor of a IBG semiconductor is lower.
4	Example of DBG semiconductor material is Gallium Arsenide (GaAs).	Examples of IBG semiconductors are Silicon and Germanium.
5	DBG semiconductors are always preferred over IBG for making optical sources.	The IBG semiconductors cannot be used to manufacture optical sources.

No	Direct Band gap semiconductor	Indirect band gap semiconductor
6	The probability of a radiative recombination is high.	The probability of a radiative recombination is comparatively low.
7	 A graph showing energy (E) on the vertical axis and wave vector (k) on the horizontal axis. Two parabolic bands are shown: a lower red band labeled 'holes' and an upper red band labeled 'electrons'. The two bands touch at the center of the Brillouin zone (k=0). A double-headed vertical arrow between the bands is labeled 'Energy gap'.	 A graph showing energy (E) on the vertical axis and wave vector (k) on the horizontal axis. Two parabolic bands are shown: a lower red band labeled 'holes' and an upper red band labeled 'electrons'. The two bands do not touch at the center of the Brillouin zone (k=0). A double-headed vertical arrow between the bands is labeled 'Energy gap'.



DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

18PYB103J –Semiconductor Physics

**Concept of phonons
Concept of Brillouin Zone (1D)
Lecture 8**

Concept of Brillouin zone

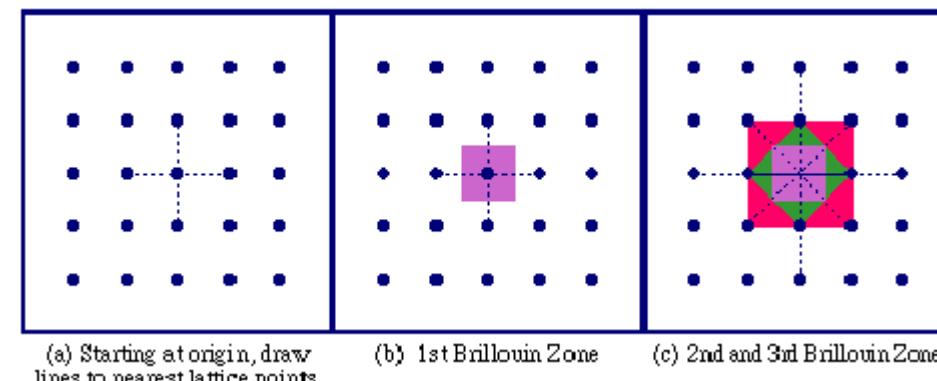


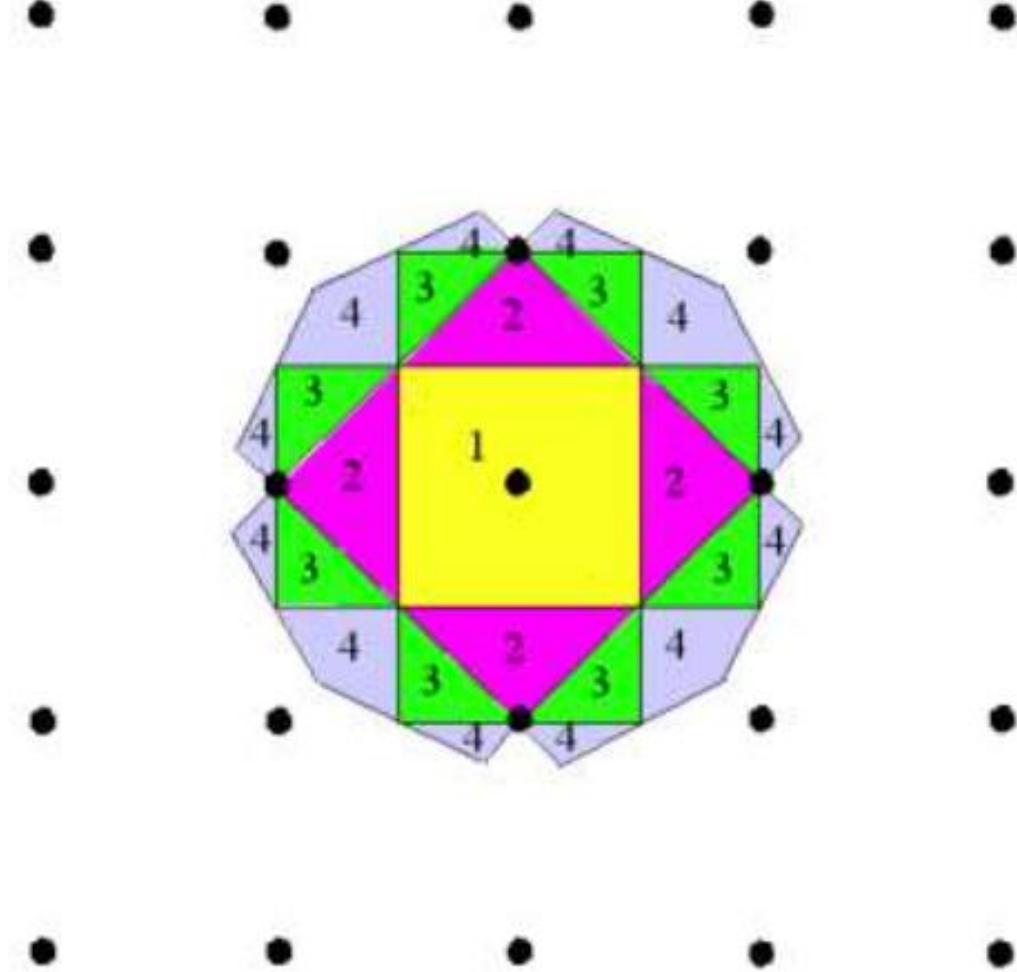
- The different Brillouin zones correspond to primitive cells of a different type that come up in the theory of electronic levels in a periodic potential.
- The first Brillouin zone is considered as the Wigner-Seitz (WS) primitive cell in the reciprocal lattice. In other words, the first Brillouin zone is a geometrical construction to the WS primitive cell in the k-space.
- In a direct lattice, **the procedure of drawing a WS cell is as follows:**
 - i) Draw lines to connect a given lattice point to all nearby lattice points.
 - ii) Draw new lines or plane at the mid point and normal to the lines.
 - iii) The smallest volume enclosed in this way is the WS primitive cell.



Remarks:

- The planes divide the Fourier space of the crystal into fragments as shown for a square lattice.
- The central square is a primitive cell of the reciprocal lattice. It is a Wigner-Seitz cell of the reciprocal lattice (called the first Brillouin zone).
- The first Brillouin zone is the smallest volume entirely enclosed by the planes.





BZ construction

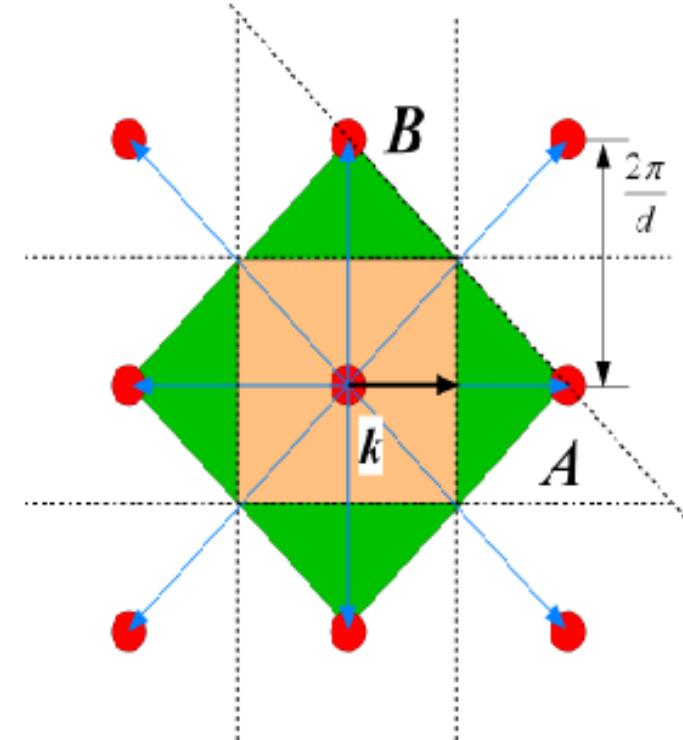
- reciprocal lattice
- bisect vectors to the nearest neighbors
- area defined by bisecting lines represents 1BZ

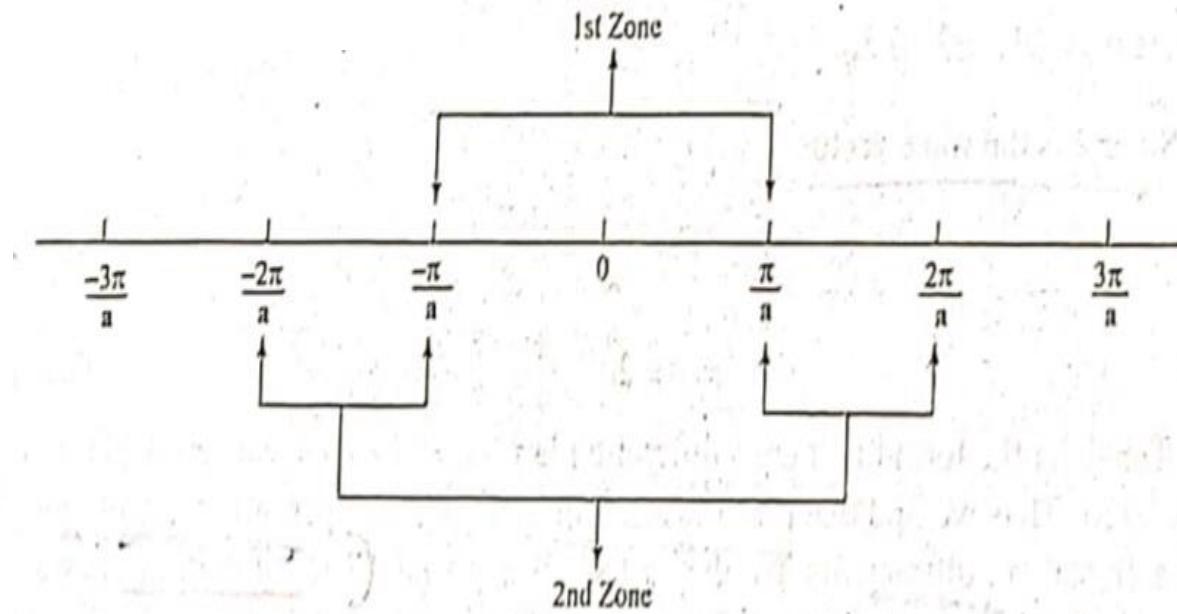
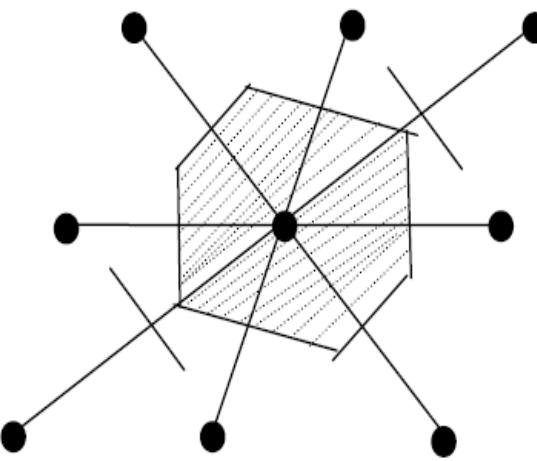
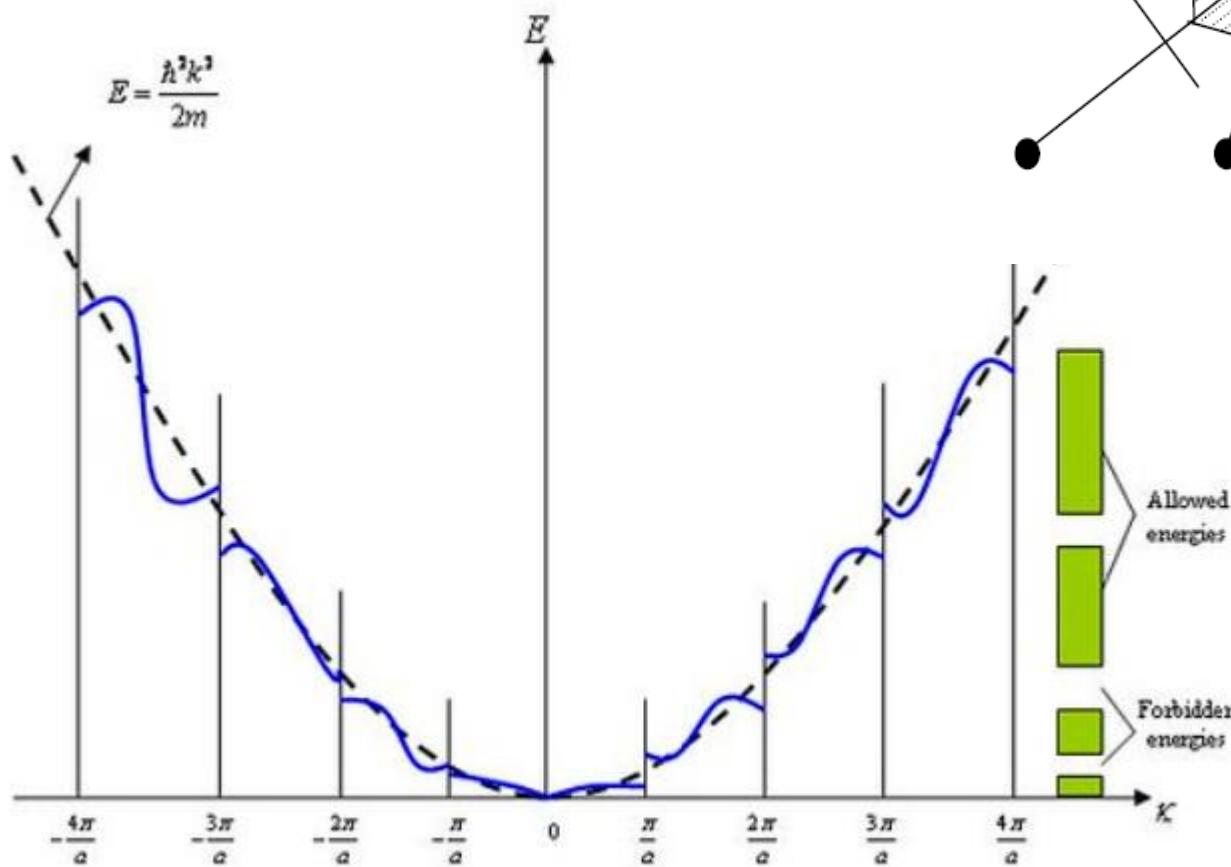


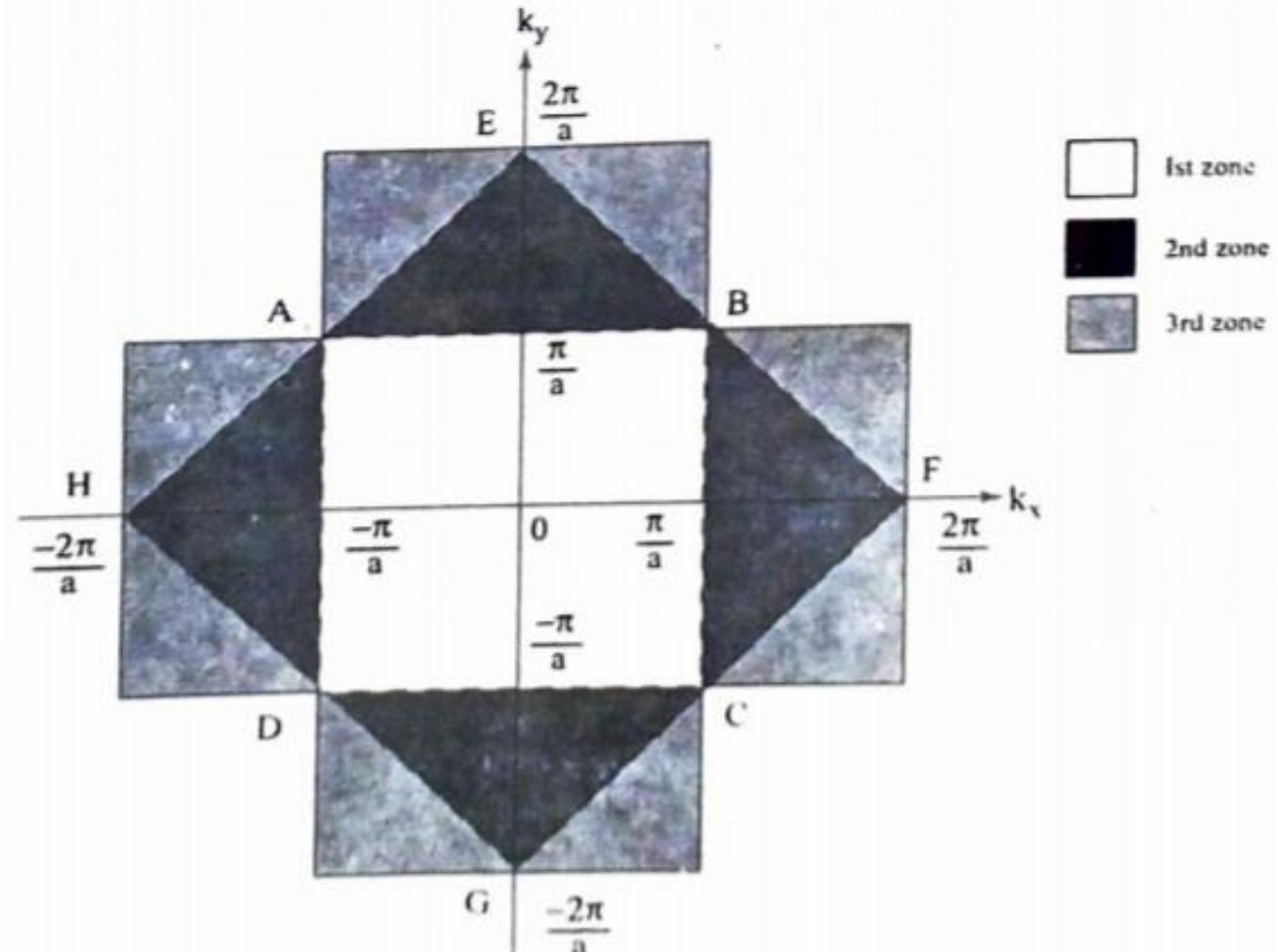
First Brillouin zone is determined

by:

- Select lattice point and draw a line segment to all neighbouring lattice points (blue).
- Draw center normal planes (black, dotted). In 2D they are lines.
- The bounded area closest to the selected point is 1. Brillouin zone (orange).
- The next area (going over one line only) is 2. Brillouin zone (green).







The first three Brillouin Zones for a two dimensional square lattice.



Conclusion:

Wigner-Seitz cell: smallest possible primitive cell, which consist of one lattice point and all the surrounding space closer to it than to any other point. The construction of the W-S cell in the reciprocal lattice delivers the first Brillouin zone (important for diffraction)

The importance of Brillouin zone:

The Brillouin zones are used to describe and analyze the electron energy in the band energy structure of crystals.

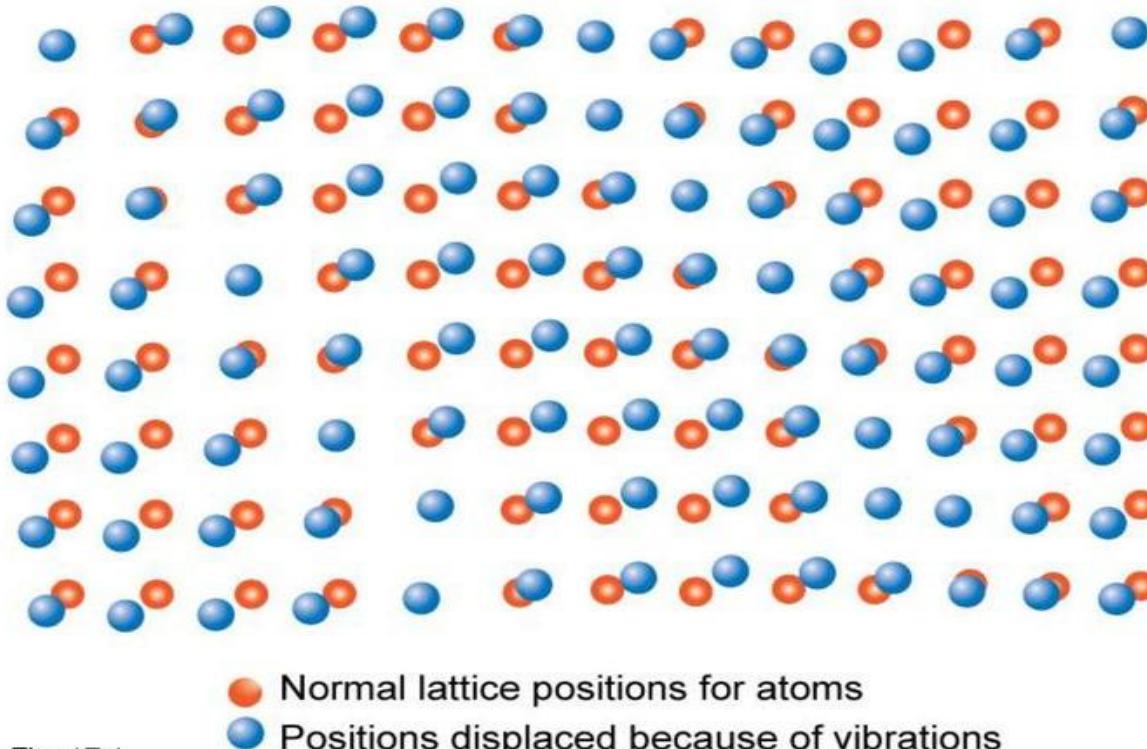
CONCEPT OF PHONONS

- Any solid crystal consists of atoms bound into a specific repeating three-dimensional spatial pattern called a lattice.
- Here the atoms behave as if they are connected by tiny springs, their own thermal energy or outside forces make the lattice vibrate.
- This generates mechanical waves that carry heat and sound through the material.
- *A packet of these waves can travel throughout the crystal with a definite energy and momentum, so in quantum mechanical terms the waves can be treated as a particle, called a phonon.*
- 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.

Concept of Phonons

Atomic Vibrations

Atomic vibrations are in the form of lattice waves or phonons



Phonon:

- ❖ A photon is the smallest unit of light. Similarly, for sound, the smallest unit is called phonon. In a lattice structure, vibrations are created by atoms. The quantized, lowest state energy of vibration is called phonon.
- ❖ Atoms were considered as rigid, with atoms stuck in their lattice. In reality, atoms can be considered as simple harmonic oscillators. The harmonic oscillator has a ground state energy and an associated vibrational mode even at 0°K .
- ❖ It is named phonons because at high energy levels long wavelength phonons give rise to sound. According to quantum mechanics, similar particles have wave nature, waves must also have particle nature. So, phonon is also treated as quasi particle. Similar to particles, these waves can carry throughout the crystal, heat, energy and momentum.



- ❖ In solid state physics, the elementary particles are electrons and phonons the arrangement of the electrons will help determine material's electrical properties whereas the speed of sound through material and heat required to change its temperature is given by phonons. Another important application of phonons is in the field of superconductivity, where the electrical resistance of certain materials become zero near absolute zero.
- ❖ In ordinary crystals, there is a loss of energy as heat as the electrons collide with impurities. But in superconductors, at low temperatures, they tend to attract slightly because of phonons. Now the movement occur as a coherent group thus minimizing energy loss.
- ❖ Phonons also have important application in detectors like Cryogenic Dark Matter Search, which aim to detect even the slightest vibration in a crystal lattice caused by even a single phonon.



Comparison between Phonons and Photons

PHONONS

- Quantized normal modes of lattice vibrations. The energies & momenta of phonons are quantized

$$E_{phonon} = \frac{h\nu_s}{\lambda}$$

$$p_{phonon} = \frac{h}{\lambda}$$

Phonon wavelength:
 $\lambda_{phonon} \approx a_0 \approx 10^{-10} \text{ m}$

PHOTONS

- Quantized normal modes of electromagnetic waves. The energies & momenta of photons are quantized

$$E_{photon} = \frac{hc}{\lambda}$$

$$p_{photon} = \frac{h}{\lambda}$$

Photon wavelength (visible):
 $\lambda_{photon} \approx 10^{-6} \text{ m}$



**DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY**

**18PY103J – Physics: Semiconductor Physics
Module-I, Lecture-9**

**ENERGY BAND STRUCTURE OF
SEMICONDUCTOR & CONCEPTS OF EFFECTIVE
MASS**

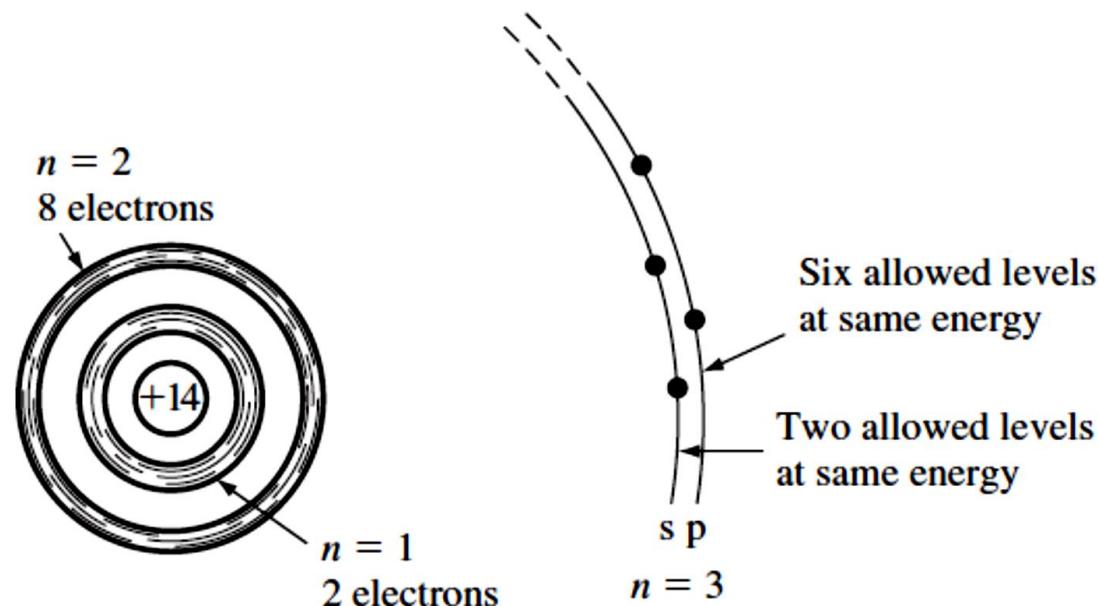


Energy Band Structure of Semiconductor Brillouin zone



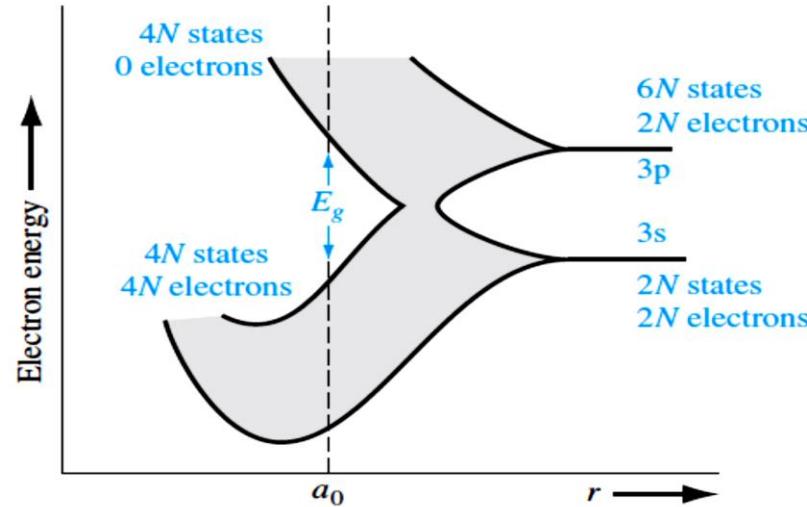
To understand the Energy band structure, consider silicon atom. A schematic representation of an isolated silicon atom is shown in Figure.

Ten of the 14 silicon atom electrons occupy deep-lying energy levels close to the nucleus. The four remaining valence electrons are relatively weakly bound and are the electrons involved in chemical reactions.





Energy Band Structure of Semiconductor Brillouin zone



Above Figure shows the band splitting of silicon. We need only to consider the $n=3$ level for the valence electrons, since the first two energy shells are completely full and are tightly bound to the nucleus.

The 3s state corresponds to $n=3$ and $l=0$ and contains two quantum states per atom. This state will contain two electrons at $T= 0$ K. The 3p state corresponds to $n= 3$ and $l=1$ and contains six quantum states per atom. This state will contain the remaining two electrons in the individual silicon atom.



As the interatomic distance decreases, the 3s and 3p states interact and overlap (*covalent bonding and crystal formation*).

At the equilibrium interatomic distance, the bands have again split, but now four quantum states per atom are in the lower band and four quantum states per atom are in the upper band.

At absolute zero degrees, electrons are in the lowest energy state, so that all states in the lower band (the valence band) will be full and all states in the upper band (the conduction band) will be empty.

The **bandgap energy** E_g between the top of the valence band and the bottom of the conduction band is the width of the forbidden energy band.



Energy Band Structure of Semiconductor Brillouin zone



At $T = 0 \text{ K}$, the $4N$ states in the lower band, the valence band, are filled with the valence electrons. All of the valence electrons are in the valence band. The upper energy band, the conduction band, is completely empty at $T = 0 \text{ K}$.

As the temperature increases above 0 K , a few valence band electrons may gain enough thermal energy to break the covalent bond and jump into the conduction band.

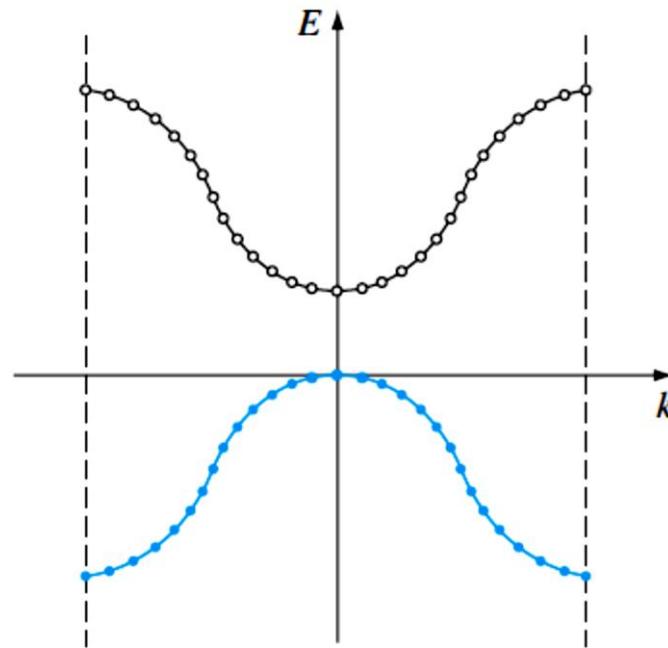
This means that, as the negatively charged electron breaks away from its covalent bonding position, a positively charged “empty state” is created in the original covalent bonding position in the valence band.

As the temperature further increases, more covalent bonds are broken, more electrons jump to the conduction band, and more positive “empty states” are created in the valence band.



This bond breaking can be related to the E versus k energy bands(first brillouin zone).

Figure shows the E versus k diagram of the conduction and valence bands at $T=0$ K. The energy states in the valence band are completely full and the states in the conduction band are empty.

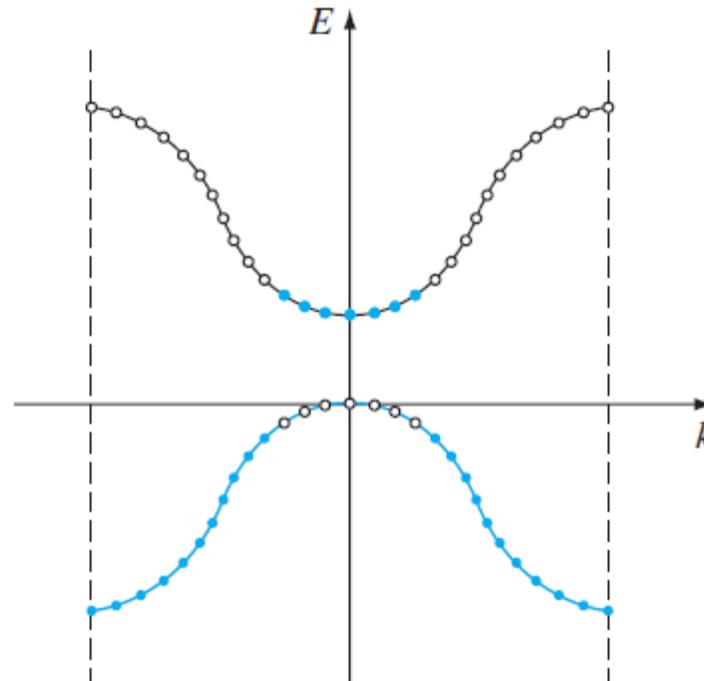




Energy Band Structure of Semiconductor Brillouin zone



Below Figure shows these same bands for $T > 0$ K, in which some electrons have gained enough energy to jump to the conduction band and have left empty states in the valence band.



The movement of an electron in a lattice will, in general, be different from that of an electron in free space.

In addition to an externally applied force, there are internal forces in the crystal due to positively charged ions or protons and negatively charged electrons, which will influence the motion of electrons in the lattice.

Then

$$F_{\text{total}} = F_{\text{ext}} + F_{\text{int}} = ma \quad (1)$$

where F_{total} , F_{ext} , and F_{int} are the total force, the externally applied force, and the internal forces, respectively, acting on a particle in a crystal. The parameter a is the acceleration and m is the rest mass of the particle.

Since it is difficult to take into account all of the internal forces, the equation becomes

$$F_{ext} = m^*a \quad (2)$$

where the acceleration a is now directly related to the external force. The parameter **m^* , called the effective mass, takes into account the particle mass and also takes into account the effect of the internal forces.**

To use an analogy for the effective mass concept, consider the difference in motion between a glass marble in a container filled with water and in a container filled with oil. In general, the marble will drop through the water at a faster rate than through the oil. The external force in this example is the gravitational force and the internal forces are related to the viscosity of the liquids. Because of the difference in motion of the marble in these two cases, the mass of the marble would appear to be different in water than in oil.



The effective mass of an electron in a crystal can be related to the E versus k curves. E-k curves of semiconductor material contains allowed energy bands that are almost empty of electrons and other energy bands that are almost full of electrons.

Recalling Equation, the energy and momentum are related by

$$E = p^2/2m = \hbar^2k^2/2m \quad (3)$$

where m is the mass of the electron. The momentum p and wave number k are related by $p=\hbar k$. Taking the derivative of Equation (3) with respect to k,

$$dE/dk = \hbar^2k/m = \hbar p/m \quad (4)$$

Relating momentum to velocity, Equation (4) can be written as

$$(1/\hbar)(dE/dk) = p/m = v \quad (5)$$

where v is the velocity of the particle. The first derivative of E with respect to k is related to the velocity of the particle.

If we now take the second derivative of E with respect to k, we have

$$d^2E/dk^2 = \hbar^2/m \quad (6)$$

Equation (6) can be rewritten as

$$(1/\hbar^2)d^2E/dk^2 = 1/m^* \quad (7)$$

The second derivative of E with respect to k is inversely proportional to the mass of the particle. For the case of a free electron, the mass is a constant (non relativistic effect), so the second derivative function is a constant.

If we apply an electric field to the free electron and use Newton's classical equation of motion, then

$$F_{ext} = m^* a = eE \quad (8)$$

where a is the acceleration, E is the applied electric field, and e is the magnitude of the electronic charge.



The effective mass is a parameter that relates the quantum mechanical results to the classical force equations.

In most instances, the electron in the bottom of the conduction band can be thought of as a classical particle whose motion can be modeled by Newtonian mechanics, provided that the internal forces and quantum mechanical properties are taken into account through the effective mass.

If we apply an electric field to the electron in the bottom of the allowed energy band, then the acceleration is

$$a = eE/m^* \quad (9)$$

where m^* is the effective mass of the electron.



**DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
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**18PY103J – Physics: Semiconductor Physics
Module-I, Lecture-13**

Classification of Electronic Materials and Fermi level



Classification of electronic materials

Conductors

Semiconductors

Insulators

Superconductor

Conductors

Conductors are substances which have free electrons, which can move under the action of an electric field. The electrons are free in the sense that they belong to the crystal as a whole and not tied down (bound) to a particular atom or a molecule. It having infinite conductivity.

Example : copper , silver etc.



Semiconductors

Semiconductors are materials which have the conductivity between conductors and insulators. Semiconductors are the elements of group-III, group-IV and group-V elements.

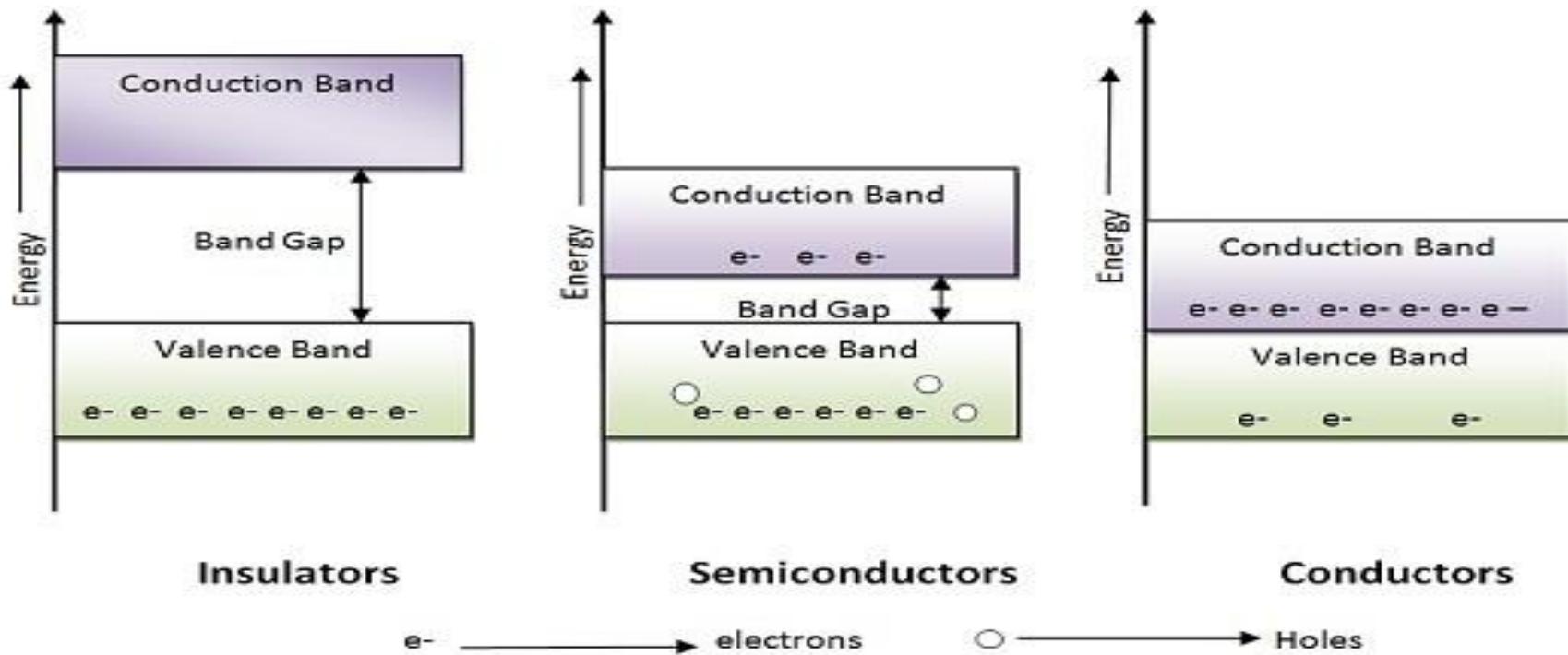
At normal temperature the conductivity of semiconductor is very low. With increase in temperature the conductivity of semiconductors increases exponentially.

Example: Germanium, Silicon, Gallium Arsenic etc.

Insulators

Insulators are very poor conductor of electricity. The forbidden gap value is $3eV$

Example: wood ,oil, mica.





This statistics applicable to the identical, indistinguishable particles of half spin.

These particles obey Pauli's exclusion principle and are called fermions
(e.g.) Electrons, protons, neutrons ...,

In such system of particles, not more than one particle can be in one quantum state.

Fermi Dirac Distribution Law is

$$n_i = \frac{g_i}{(e^{\alpha + \beta E_i}) + 1}$$

Fermi Energy



Fermi Energy (E_F)

Fermi Energy is the energy of the state at which the probability of electron occupation is $\frac{1}{2}$ at any temperature above 0 K.

It is also the maximum kinetic energy that a free electron can have at 0 K.

The energy of the highest occupied level at absolute zero temperature is called the *Fermi Energy or Fermi Level*.

Fermi Energy



The Fermi energy at 0 K for metals is given by

$$E_F = \left[\frac{3N}{\pi} \right]^{2/3} \left(\frac{\hbar^2}{8m} \right)$$

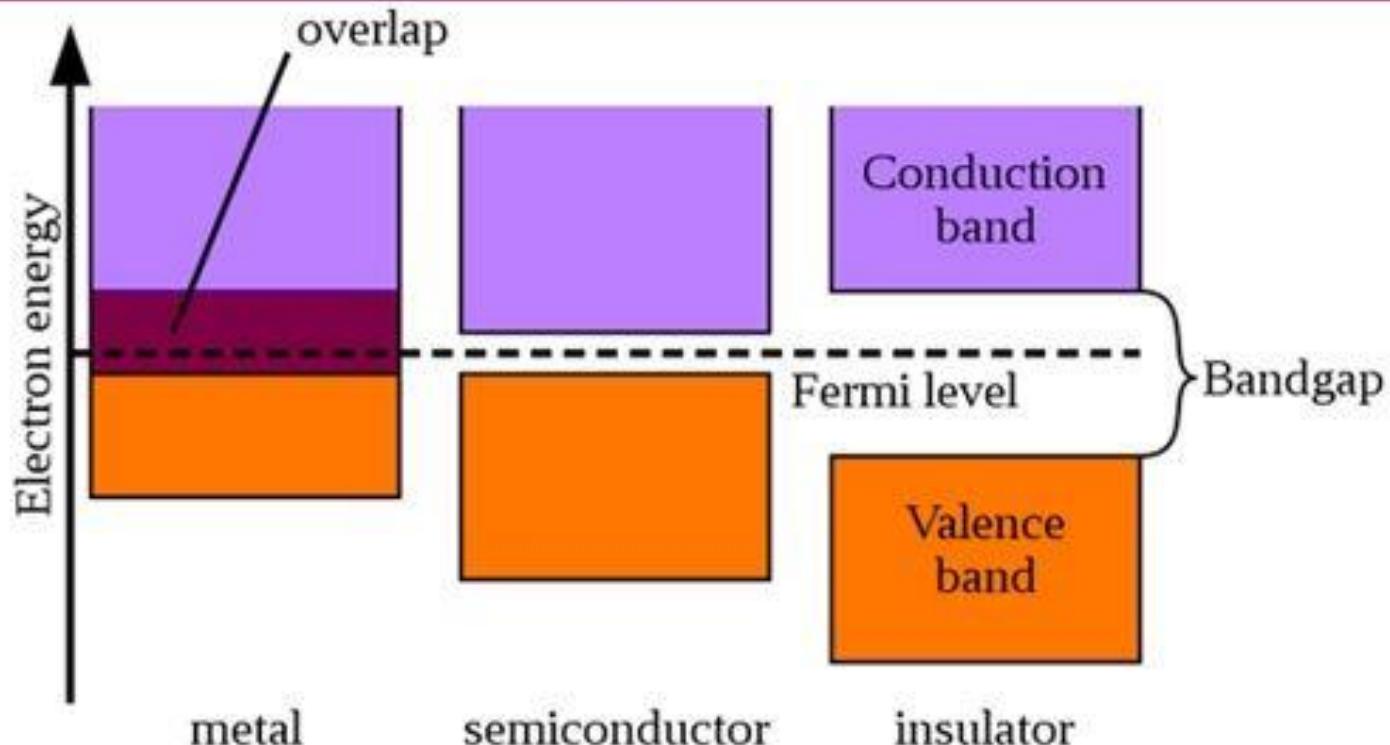
When temperature increases, the Fermi level or Fermi energy also slightly decreases.

The Fermi energy at non-zero temperatures,

$$E_F = E_{F_0} \left[1 - \frac{\pi^2}{12} \left(\frac{kT}{E_{F_0}} \right)^2 \right]$$

Here the subscript ‘0’ refers to the quantities at zero kelvin

FERMI ENERGY





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**18PY103J – Physics: Semiconductor Physics
Module-I, Lecture-14**

Fermi-Dirac Distribution Function $f(E)$ and Influence of donors in semiconductors



The free electron gas in a solid obeys Fermi-Dirac statistics.

Suppose in an assemblage of fermions, there are $M(E)$ allowed quantum states in an energy range between E and $E+dE$ and $N(E)$ is the number of particles in the same range.

The Fermi-Dirac distribution function is defined as,

$$\frac{N(E)}{M(E)} = \frac{1}{1 + \exp((E - E_F)/kT)}$$

$N(E) / M(E)$ is the fraction of the possible quantum states which are occupied.



The distribution of electrons among the levels is described by function $f(E)$, *probability of an electron occupying an energy level ' E '*.

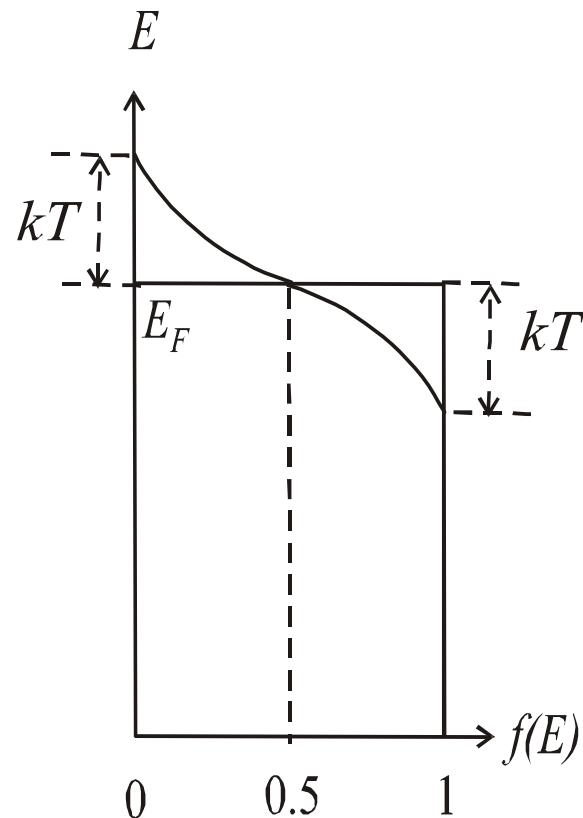
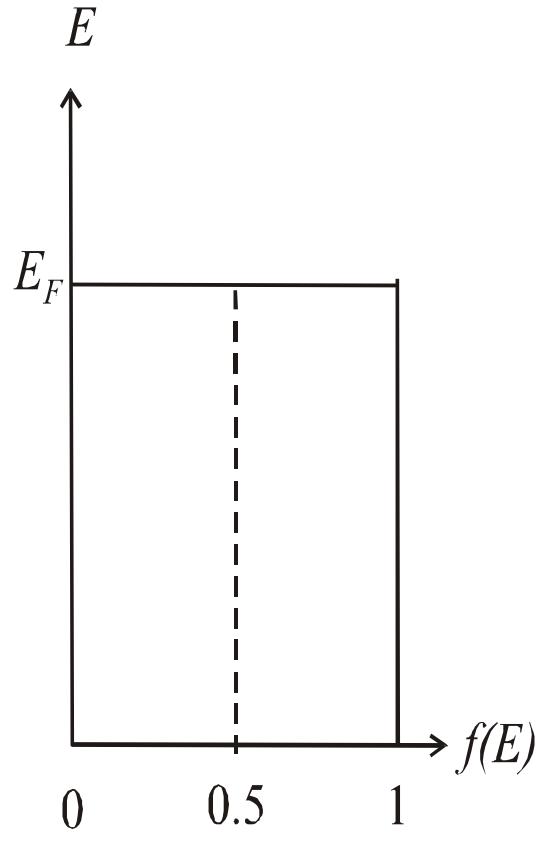
If the level is certainly empty, then $f(E) = 0$. Generally the $f(E)$ has a value in between zero and unity.

When $E < E_F$ (i.e.,) for energy levels lying below E_F , $(E - E_F)$ is a negative quantity and hence,

$$f(E) = \frac{1}{1 + e^{-\infty}} = \frac{1}{1 + 0} = 1$$

That means all the levels below E_F are occupied by the electrons.

Fermi-Dirac Distribution Function $f(E)$



Fermi Dirac distribution function at different temperatures



When $E > E_F$ (i.e.) for energy levels lying above E_F , $(E - E_F)$ is a positive quantity

$$f(E) = \frac{1}{1 + e^{\infty}} = \frac{1}{1 + \infty} = 0$$

This equation indicates all the levels above E_F are vacant.

At absolute zero, all levels below E_F are completely filled and all levels above E_F are completely empty.

This level, which divides the filled and vacant states, is known as the Fermi energy level.



When $E = E_F$,

$$f(E) = \frac{1}{1 + e^0} = \frac{1}{1+1} = \frac{1}{2} \quad \text{at all temperatures}$$

The probability of finding an electron with energy equal to the Fermi energy in a metal is $\frac{1}{2}$ at any temperature.

At $T = 0$ K all the energy level upto E_F are occupied and all the energy levels above E_F are empty .

When $T > 0$ K, some levels above E_F are partially filled while some levels below E_F are partially empty.



The group V element has five valence electrons. Four of these will contribute to the covalent bonding with the silicon atoms, leaving the fifth more loosely bound to the phosphorus atom. the fifth valence electron as a donor electron.

The phosphorus atom without the donor electron is positively charged.

At very low temperatures, the donor electron is bound to the phosphorus atom.

However By intuition, it should seem clear that the energy required to elevate the donor electron into the conduction band is considerably less than that for the electrons involved in the covalent bonding.



If a small amount of energy, such as thermal energy, is added to the donor electron, it can be elevated into the conduction band, leaving behind a positively charged phosphorus ion.

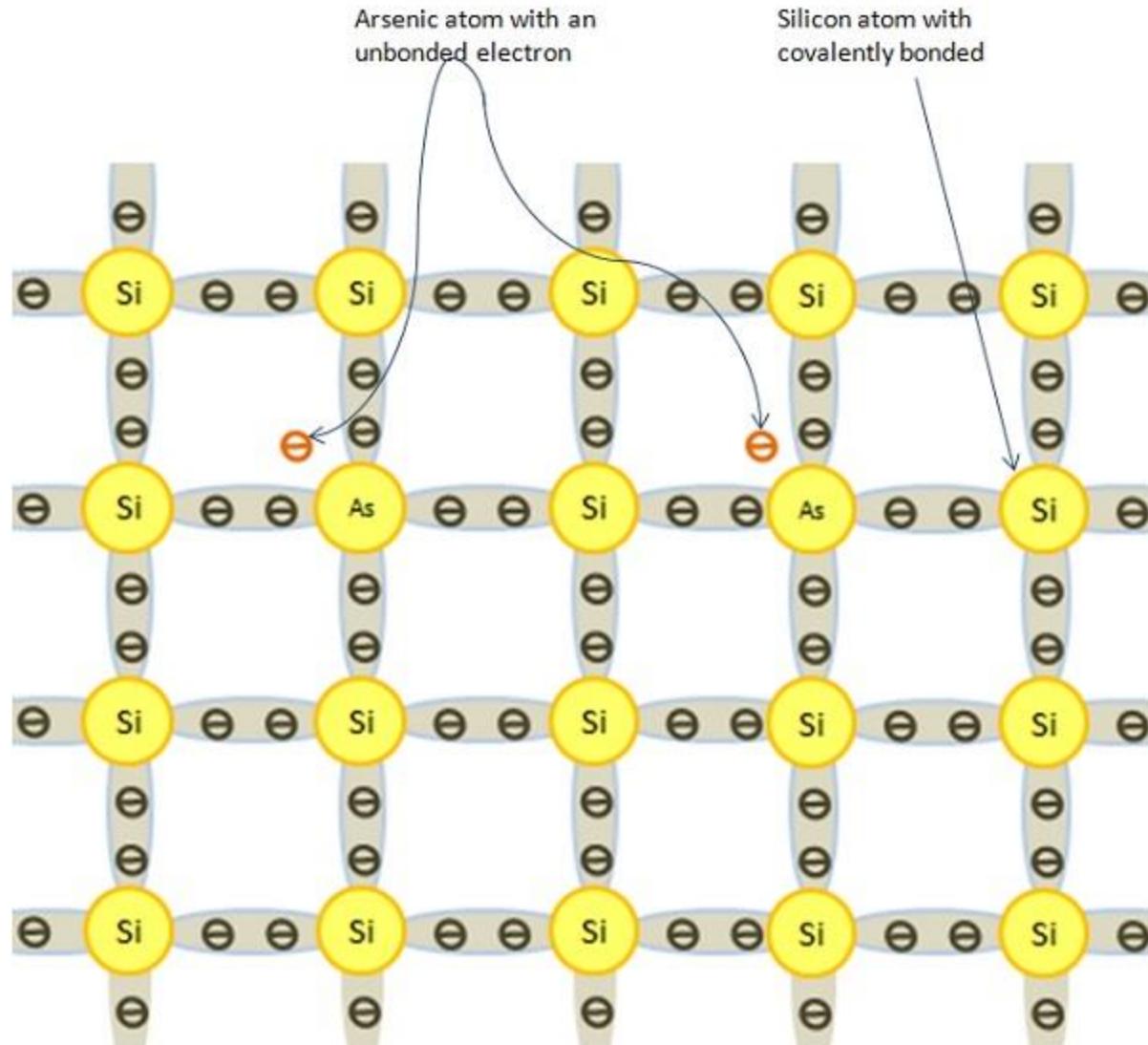
The electron in the conduction band can now move through the crystal generating a current, while the positively charged ion is fixed in the crystal.

This type of impurity atom donates an electron to the conduction band and so is called a *donor impurity atom*.

The donor impurity atoms add electrons to the conduction band without creating holes in the valence band. The resulting material is referred to as an n -type semiconductor (n for the negatively charged electron)



Influence of donors in semiconductors



Influence of donors in semiconductors

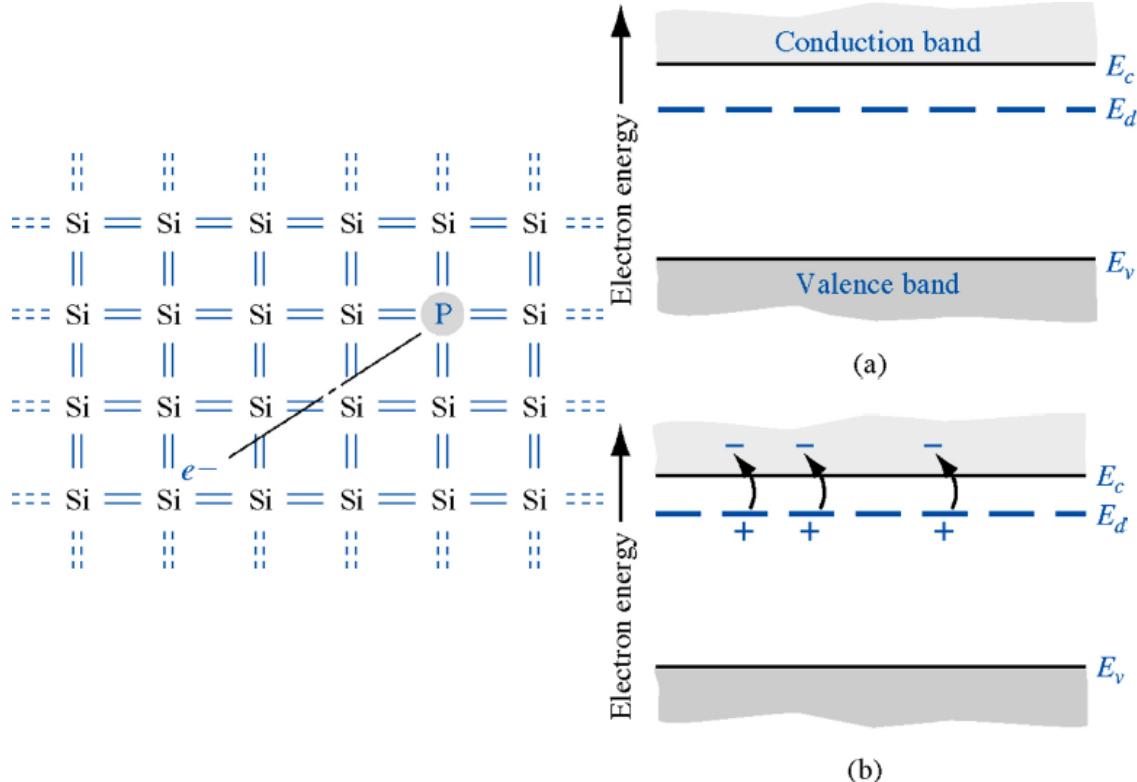


Figure shows the energy-band diagram that we would expect. The energy level, E_d , is the energy state of the donor electron.



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**18PY103J – Physics: Semiconductor Physics
Module-I, Lecture-15**

Influence of Acceptor in Semiconductors

Influence of acceptor in semiconductors

- Consider adding a group III element, such as boron, as a substitutional impurity to silicon. The group III element has three valence electrons, which are all taken up in the covalent bonding. As shown in Figure a.
- one covalent bonding position appears to the empty. If an electron were to occupy this "empty" position its energy would have to be greater than that of the valence electrons, since the net charge state of the boron atom would now be negative.
- However, the electron occupying this "empty" position does not have sufficient energy in the conduction band, so its energy is far smaller than the conduction-band energy.

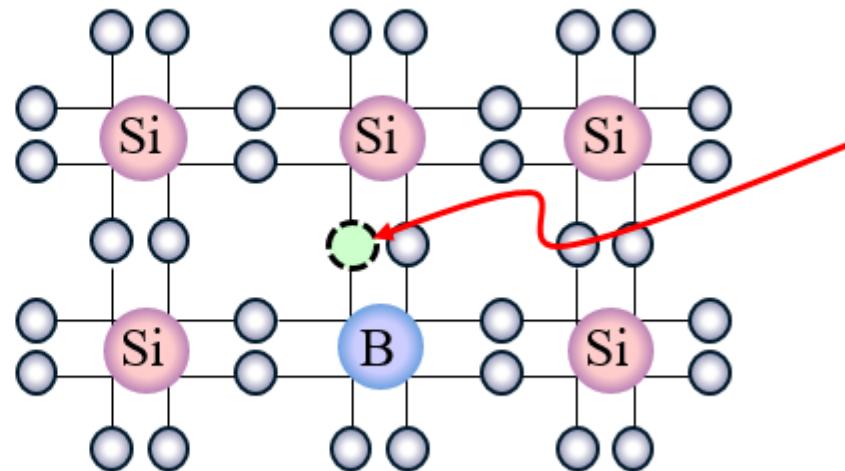
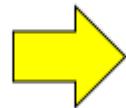
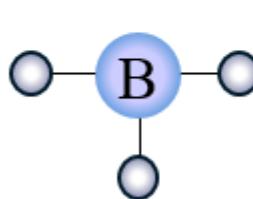
Influence of acceptor in semiconductors

- The "empty" position associated with the boron atom becomes occupied, and other valence electron positions become vacated. These other vacated electron positions can be thought of as holes in the semiconductor material.
- Figure b. shows the expected energy state of the "empty" position and also the formation of a hole in the valence band. The hole can move through the crystal generating a current, while the negatively charged boron atom is fixed in the crystal.
- The group III atom accepts an electron from the valence band and so is referred to as acceptor impurity). atom. The acceptor atom can generate holes in the valence band without generating electrons in the conduction band. This type of semiconductor material is referred to as a p-type material (*p for the positively charged hole*).



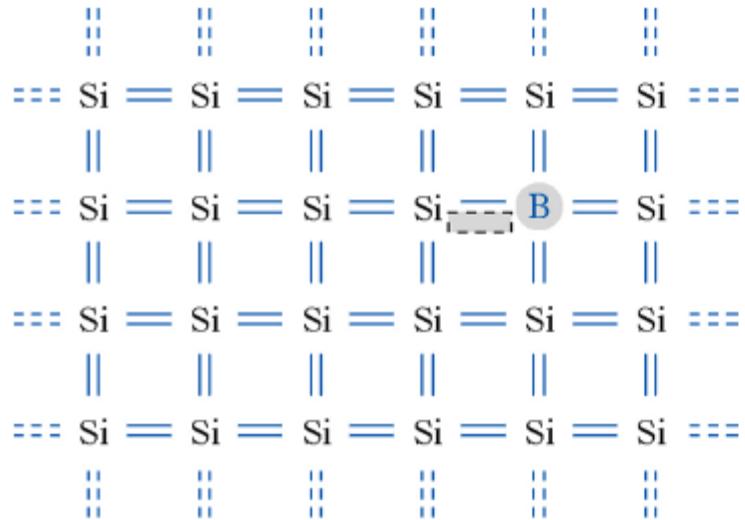
Influence of acceptor in semiconductors

p-type semiconductor

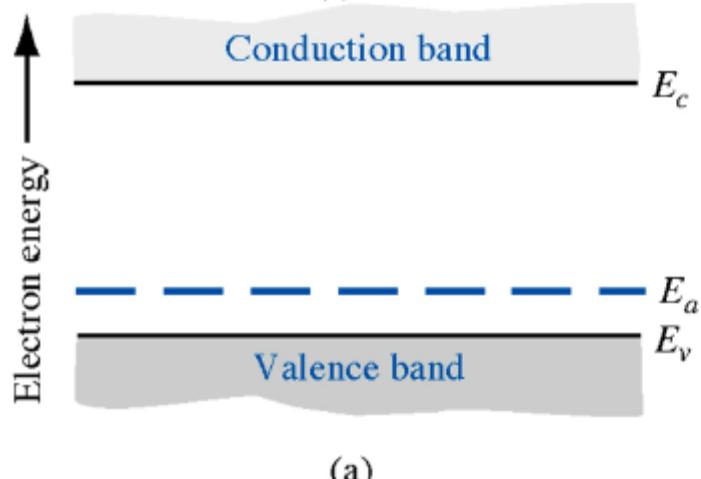




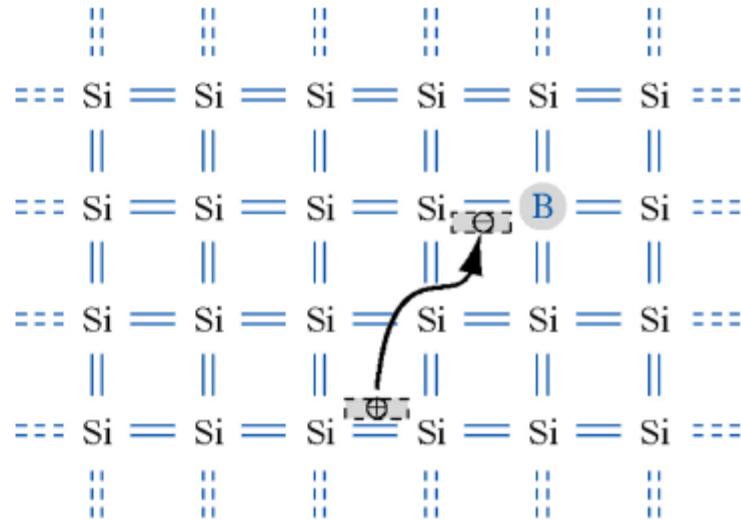
Influence of acceptor in semiconductors



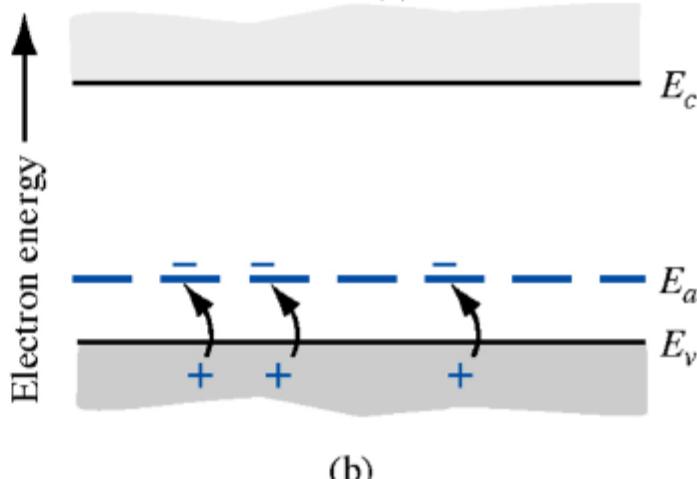
(a)



(a)



(b)



(b)



we have only considered the thermal equilibrium carrier densities, n_o and p_o . However most devices of interest are not in thermal equilibrium. Keep in mind that a constant ambient constant temperature is not a sufficient condition for thermal equilibrium.

In fact, applying a non-zero voltage to a device or illuminating it with light will cause a non-equilibrium condition, even if the temperature is constant.

To describe a system that is not in thermal equilibrium we assume that each of the carrier distributions is still in equilibrium with itself. Such assumption is justified on the basis that electrons readily interact with each other and interact with holes only on a much longer time scale.



The electron density can still be calculated using the Fermi-Dirac distribution function, but with a different value for the Fermi energy. The total carrier density for a non-degenerate semiconductor is then described by:

$$n = n_o + \delta n = n_i \exp\left(\frac{F_n - E_i}{kT}\right)$$

Where δn is the *excess electron density* and F_n is the *quasi-Fermi energy* for the electrons. Similarly, the hole density can be expressed as:

$$p = p_o + \delta p = n_i \exp\left(\frac{E_i - F_p}{kT}\right)$$

Where δp is the *excess hole density* and F_p is the *quasi-Fermi energy* for the holes.



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**18PY103J – Physics: Semiconductor Physics
Module-I, Lecture-16**

Numericals Based on Fermi Level and Fermi Distribution Function

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

Solution:-

We have the formula, $E_F = 1/2 m v_F^2$

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

$$= ((2 \times 2.1 \times 1.602 \times 10^{-19}) / 9.11 \times 10^{-31})^{1/2}$$

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

2 . Evaluate the Fermi function for energy $K_B T$ above the Fermi energy.

Solution:

We know Fermi Function $F(E) = \frac{1}{1 + e^{(E - E_F)K_B T}}$

For an energy $K_B T$ above Fermi energy

$$E - E_F = K_B T$$

$$F(E) = \frac{1}{1 + e^1} = \frac{1}{1 + 2.7183}$$

Fermi distribution function $F(E) = 0.2689$

3. The Fermi temperature of a metal is 24600 K. Calculate the Fermi velocity.

Solution:

Given data:

$$\text{Temperature} = 24600 \text{ K}$$

The relation between Fermi energy, Fermi velocity and Fermi temperature is given by

$$E_F = \frac{3}{2} K_B T_F = \frac{1}{2} m V_F^2$$

$$V_F = \sqrt{\frac{3K_B T_F}{m}} = \sqrt{\frac{31.38 \times 10^{-23} \times 24600}{9.11 \times 10^{-31}}}$$

Fermi velocity

$$V_F = 863.30 \times 10^3 \text{ ms}^{-1}$$



4. Use the Fermi distribution function to obtain the value of $F(E)$ for $E - E_F = 0.01 \text{ eV}$ at 200K.

Given data:

$$\text{Fermi Function} \quad F(E) = \frac{1}{1 + e^{(E - E_F)/K_B T}}$$

$$\text{Boltzman constant} \quad K_B = 1.38 \times 10^{-23} \text{ JK}^{-1}$$

$$E - E_F = 0.01 \text{ eV} = 0.01 \times 1.6 \times 10^{-19} = 1.6 \times 10^{-21} \text{ J}$$

$$T = 200 \text{ K}$$

$$F(E) = \frac{1}{1 + e^{1.6 \times 10^{-21} / (1.38 \times 10^{-23} \times 200)}}$$

$$= \frac{1}{1 + e^{0.5797}}$$

$$= \frac{1}{1 + 1.7855} = \frac{1}{2.7855}$$

Fermi function

$$F(E) = 0.3589$$