DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

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.

C.B

E_g

V.B
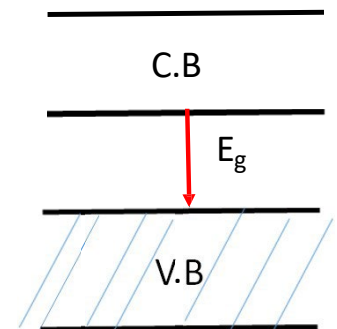
- Most of the semiconductors are in crystalline form, i.e the atoms are arranged in periodic manner.
- The motion of electron in a crystal is governed by the laws of quantum mechanics.
- If we have one electron and one proton system like hydrogen atom it is easy to solve Schrodinger equation.
- But in 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 $|\Psi|^2$

$PE(r)$
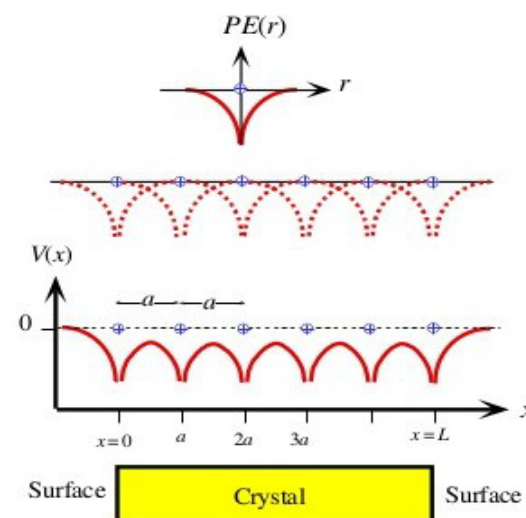
PE of the electron around an isolated atom

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

$V(x)$

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

Surface | Crystal | Surface

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

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

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)

i.e V(x) = V (x+a)--------(2)

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

$\Psi_k(x) = e^{ikx}u_k(x)$--------(3), where $u_k(x) = u_k(x + a)$ (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

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

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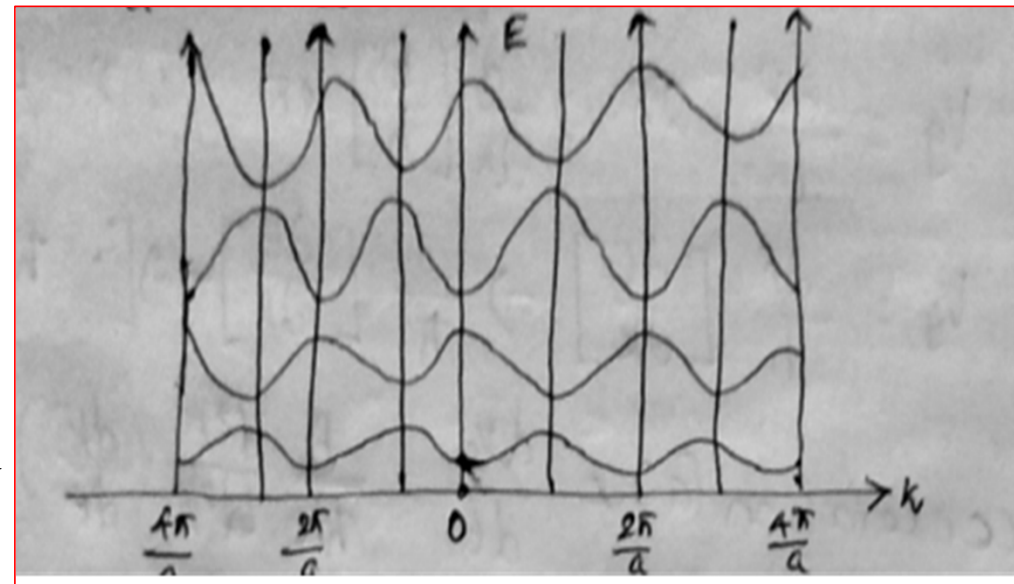
So the energy Eigen values are periodic in k space

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:

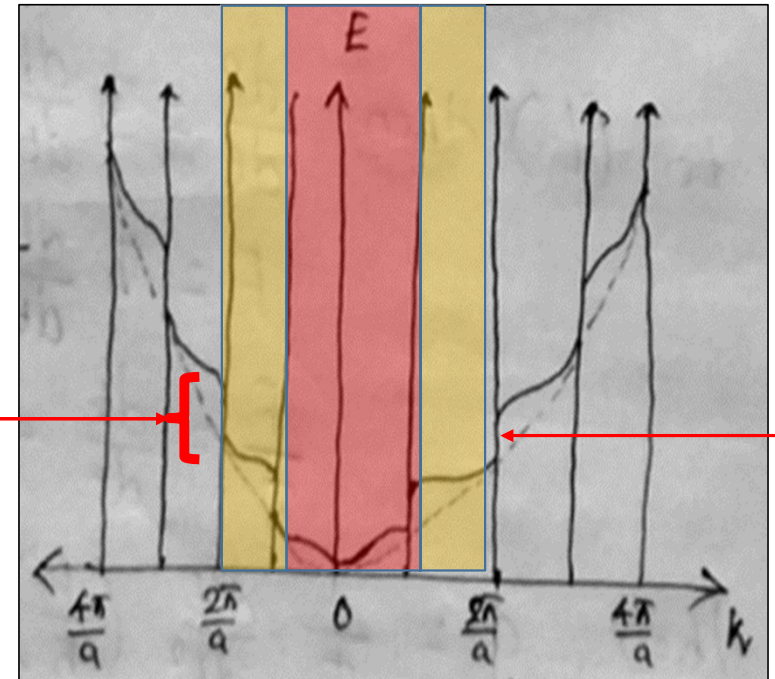In this scheme, different bands are drawn in different zones. In k- space.

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

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 :

o 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.

o **If we know the energy values of first zone with respect to K then we know every where because energy Eigen values are periodic**

o In many of optoelectronic text books the reduce zone scheme is shown

The E-k Diagram

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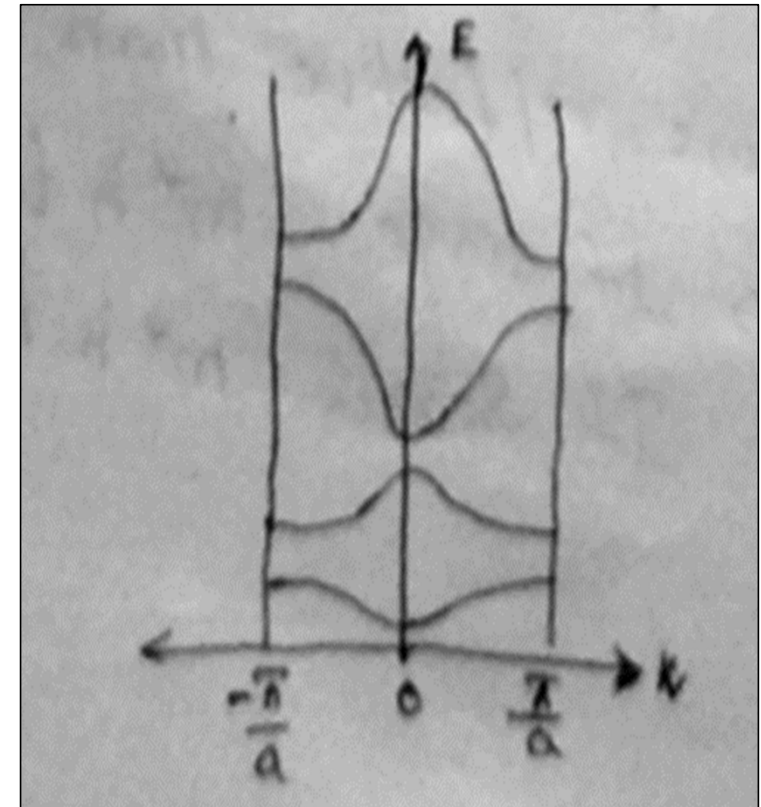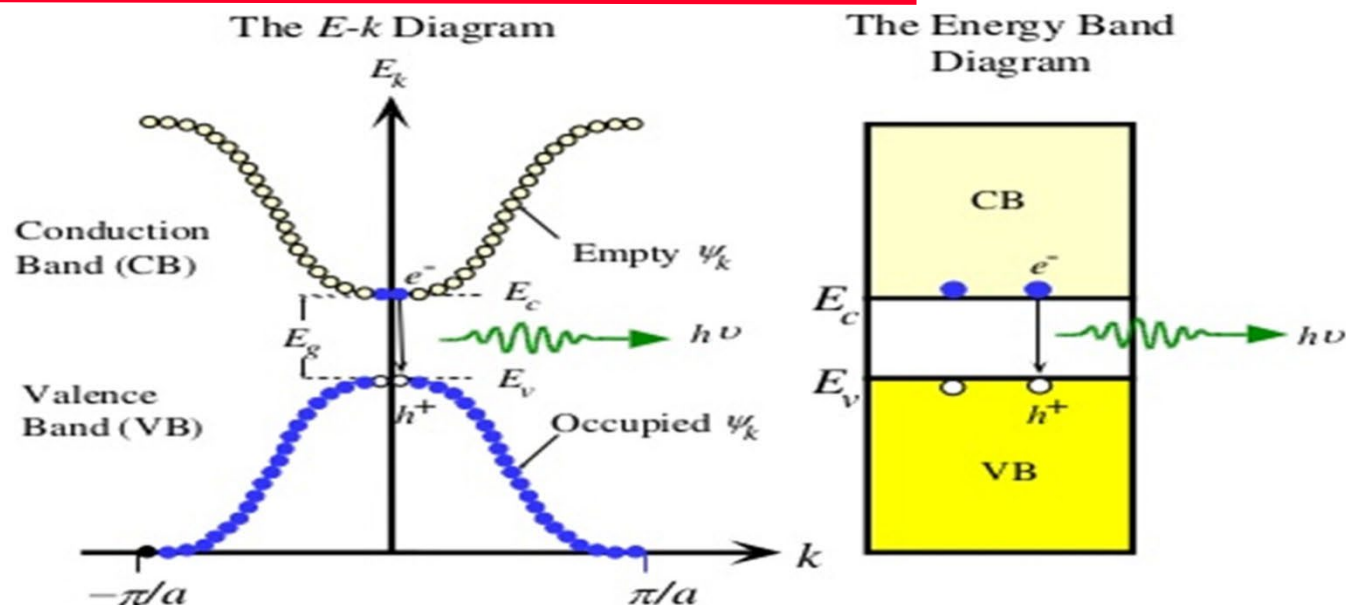
The E-k diagram of a direct bandgap semiconductor such as GaAs. The E-k curve consists of many discrete points with each point corresponding to a possible state, wavefunction $\Psi_k(x)$, that is allowed to exist in the crystal. The points are so close that we normally draw the E-k relationship as a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

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 bandgap semiconductors:

E

electrons

Energy gap

holes

k

Direct bandgap semiconductors

E

electrons

Energy gap

holes

k

Indirect bandgap semiconductors
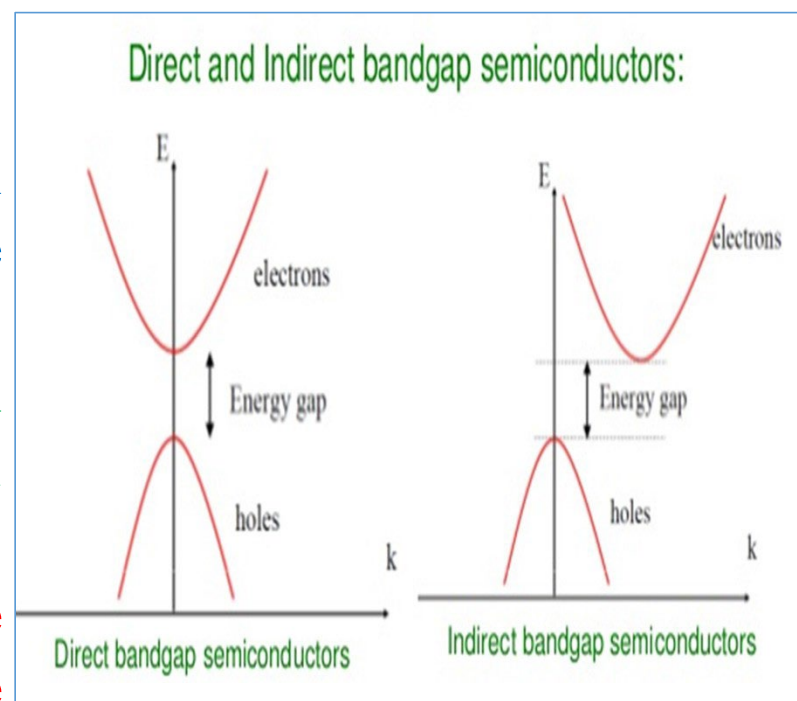
Direct and Indirect band gap semiconductors

- 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 $(K) = \dfrac{1}{2}mv^2$, and
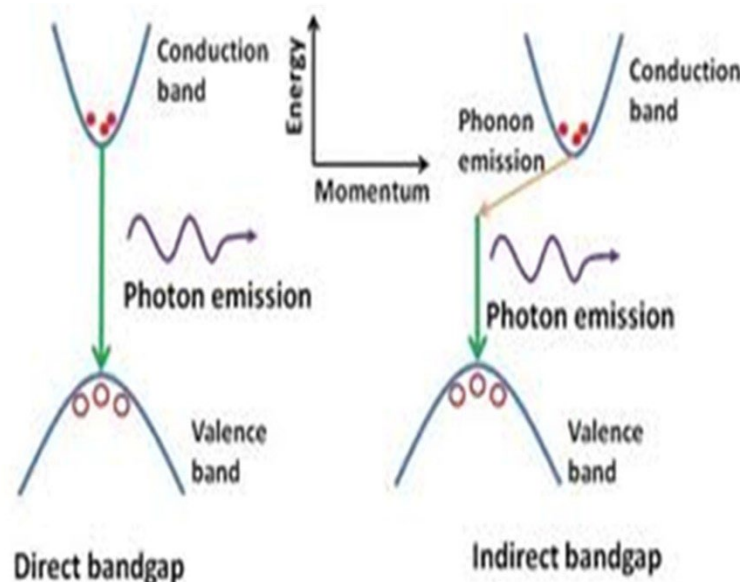
Momentum $(p) = mv$

Where, symbols have usual meaning.

Now,

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

therefore,

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

Direct bandgap — Conduction band, Photon emission, Valence band

Indirect bandgap — Conduction band, Phonon emission, Photon emission, Valence band
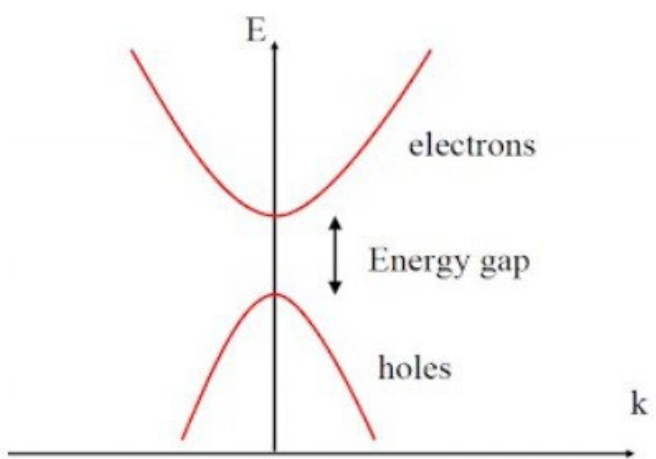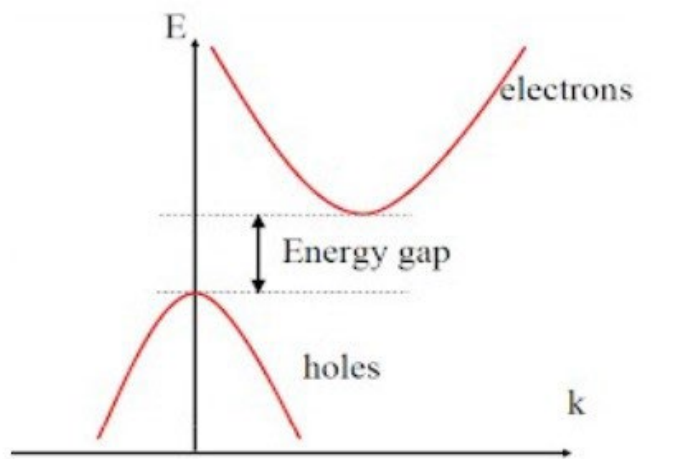
Energy / Momentum axes

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		

What is next?

Material	Energy gap (eV)		
	0K	300K	
Si	1.17	1.11	Indirect
Ge	0.74	0.66	Indirect
InSb	0.23	0.17	Direct
InAs	0.43	0.36	Direct
InP	1.42	1.27	Direct
GaP	2.32	2.25	Indirect
GaAs	1.52	1.43	Direct
GaSb	0.81	0.68	Direct
CdSe	1.84	1.74	Direct
CdTe	1.61	1.44	Direct
ZnO	3.44	3.2	Direct
ZnS	3.91	3.6	Direct

These materials are either Direct or Indirect bandgap semiconductor. Do we have materials available in which both Direct or Indirect bandgap exist?

MoS_2

Bulk MoS_2 is a semiconductor with an indirect bandgap (1.2 eV), however monolayer MoS_2 is direct bandgap (1.9 eV) semiconductor due to the 2D confinement!