MODULE- I

BAND THEORY OF SOLIDS :- 1

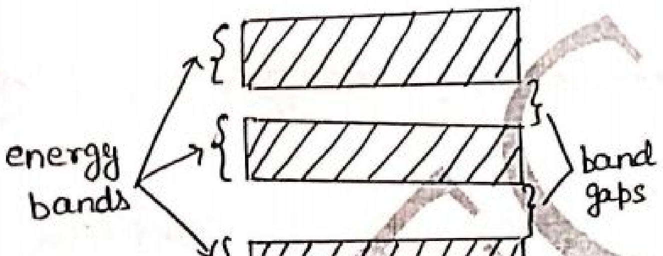
The electrical properties of many metals, semiconduc-
-tors can not be explained on the basis of free electron
theory. This can be done only by considering the electrons
to be present in a periodic potential (i.e crystal
lattice). The concept of discrete allowed electron
energies that occur in a single atom, has to be expanded
to a band of allowed energies. In this process, we
will enter into a more valid description of electrons
in a periodic lattice, namely, the energy band
theory.

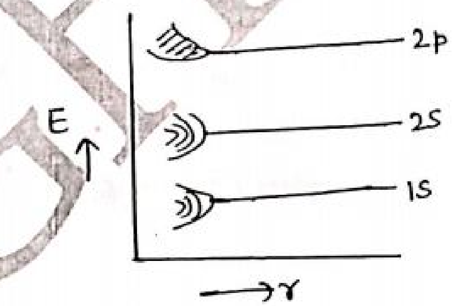
The energy band theory is now a basic principle of
semiconductor physics and is used to explain the
differences in electrical properties between metals,
insulators and semiconductors.

Due to periodicity of the lattice, each atom is in the
electrostatic field of the neighbouring atoms. Consequ-
-ently, the energy levels of an individual atom
loose their validity. If the crystal contains N-atoms,
then due to interaction between the atoms, each discrete
energy level in an individual atom splits into N-close
sublevels. As N is very large, the seperation between
sublevels is very small so that these dense levels
are almost continuous and are said to form an
energy band. These energy bands are in general,
seperated by regions which have no allowed energy
levels. These regions are called forbidden bands or
band gaps.

In some crystals, the adjacent energy bands
overlap. The no. of levels in such a merged band

is equal to the sum of the number of the levels into which both levels of the atoms split up. Moreover, the amount of splitting is not the same for different levels. Those filled up by the valence electrons in an atom are disturbed most, while those filled by inner electrons disturbed only slightly. figure represents the splitting of levels as a function of distance r between atoms. The energy band structure of a solid and the occupation of energy bands by electrons determine the electrical properties of that solid.

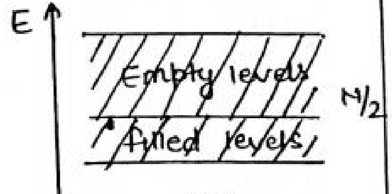




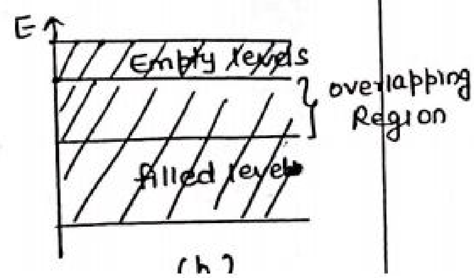
CLASSIFICATION OF SOLIDS ON THE BASIS OF ENERGY BAND GAP :-

The concept of energy bands helps us in understanding the divison of solids into three groups.

Conductor :- In some solids, an upper vacant band overlaps the valence band or the valence band itself is half-filled. It means that electrons in the valence band have easy access to levels in the upper vacant band. For this reason, very large no. of electrons



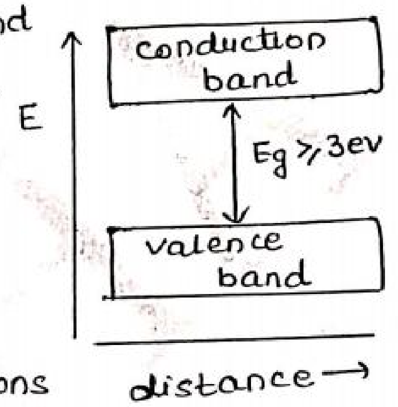
(a)



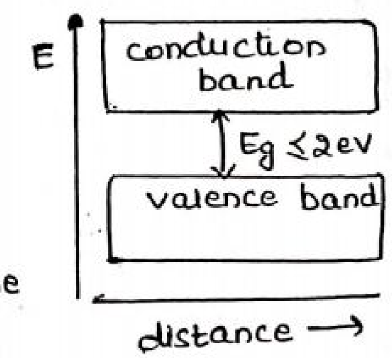
(b)

are available for conduction, even at extremely
low temperatures. when electric field is impressed
across the solid, electrons readily jump into
upper unoccupied energy levels of the vacant band
and current flows in a large measure in the
solid. Therefore, these solids exhibit good electrical
conductivity and are called <u>conductors</u>.

<u>Insulator</u> :- Some solids have band
gaps that are very wide ($E_g > 3ev$).
It would require the acquistion
of very large amounts of energy
to cause an electron to jump
from the valence band to the
conduction band. very few electrons
can get this large amount of energy
to jump from valence band to conduction band at
ambient temperature. Hence, there are very few
electrons in the conduction band. when a voltage
is applied across the solid, negligible current flows
and the solid exhibits very low electrical conducti-
-vity. These solids are called <u>insulators</u>.



<u>semiconductor</u> :- In some solids,
the band gap is narrow and
of the order of 2ev or less.
Acquistion of small amounts of
energy from the vibrations of
atom can raise electrons from the
valence band to the conduction
band. The conduction band is then partially
filled. If a potential is applied across the
material, it causes the electrons in the conduction



band to move to upper levels. As a result, current flows in a modest measure in the solid. Such solids are called <u>semiconductors</u>.

CLASSIFICATION OF SEMICONDUCTORS :-

semiconductors are classified mainly on three ways based on the composition of materials, purity of the material and nature of band gap of the material.

Semiconductor

- Based on composition
  - elemental
  - compound
- Based on impurity
  - Intrinsic
  - Extrinsic
    - P-type
    - n-type
- Based on the band gap
  - Direct band gap
  - Indirect band gap

Based on composition :-

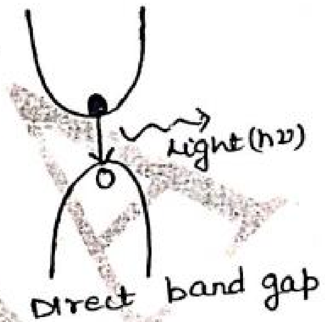
1. **Elemental Semiconductor :-** These types of semiconductors are made of a single element of fourth group elements of the periodic table.
   example : Germanium and silicon

2. **Compound Semiconductor :-** semiconductors which are formed by combining third and fifth group elements (III-V) or second and sixth group elements (II-VI) of the periodic table are known as compound semiconductors.
   for ex : GaAs, GaP, InSb, ZnS, CdS, CdTe

Based on band gap :-

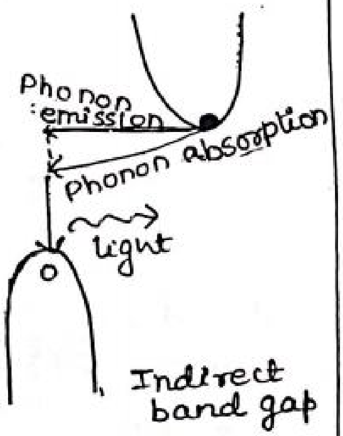
Direct band gap semiconductor :- In a direct band gap semiconductor such as GaAs, AlAs and InP, when an excited electron falls back into the valence band, the electrons and holes recombine to produce light energy.

i.e $e^- + \text{hole} \longrightarrow h\nu$ (photon)



This process is known as radiative recombination. Also called spontaneous emission. These direct band gap semiconductor are used to make LEDs and Lasers of different colours.

Indirect band gap semiconductor :- In an indirect band gap semiconductor such as Si, Ge and GaP, when an excited electron falls back into the valence band, the electron and hole recombine to generate heat and is dissipated within the material.



i.e $e^- + \text{hole} \rightarrow$ phonon.

This process is known as non-radiative recombination.

Based on Impurity :-

Intrinsic Semiconductor :- A sample of semiconductor in its purest form is called an intrinsic semiconductor. These semiconductors possess poor conductivity.

In intrinsic semiconductor, the energy band gap between valence and conduction band is relatively small. Hence, at room temperature, some electrons may possess enough thermal energy to cross over the band gap and enter the conduction band. Thus, the excited electrons leave behind a vacancy which may be filled by another electron in the valence band. The vacancy produced in the valence band due to the electron excitation is called a <u>hole</u>.

In intrinsic semiconductor for every conduction electron promoted to the conduction band, there is a hole in the valence band. Holes and electrons created in this way are known as <u>intrinsic charge carriers.</u>

Thus, in intrinsic semiconductor

$$n_e = n_h$$

i.e the density of electrons = the density of holes

In an intrinsic semiconductor, when an electron moves to fill a hole, another hole is created at the original electron source. Consequently, the holes appear to act as positively charged electron and carry an electrical charge.

When a voltage is applied to the material, the electrons in the conduction band accelerate towards the positive terminal and holes in the valence band move towards the negative terminal. Hence, current conduction takes place due to the movement of both the charge carriers electrons and holes.

Thus, conductivity

$$\sigma_i = n_e e \mu_e + n_h e \mu_h$$

or $$\boxed{\sigma_i = n_i e(\mu_e + \mu_h)}$$

$\because n_e = n_h = n_i$ ↓ Intrinsic carrier concentration

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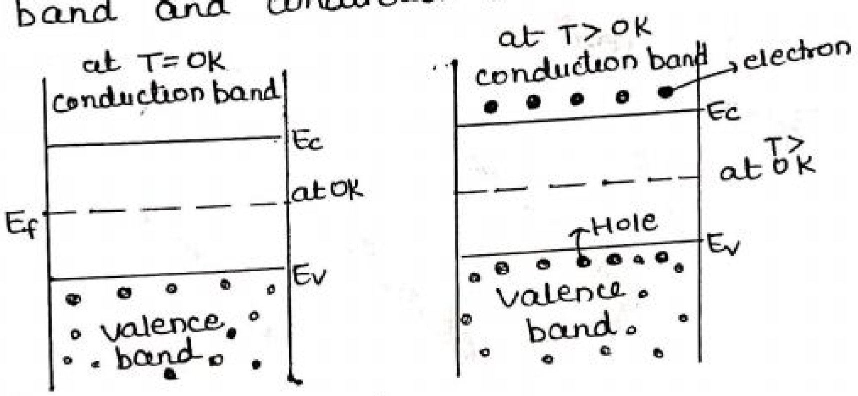
Carrier concentration in an intrinsic semiconductor:-

In general, the number of charge carriers per unit volume of the material is called carrier concentration.

At 0K, in an intrinsic S.C., the valence band is completely filled and the conduction band is completely empty. The fermi level lies exactly midway between the valance band and conduction band.



As the temperature of the semiconductor is increased, electrons from the valence band get thermally excited to the conduction band. These electrons in the conduction band behave like a free particle with an effective mass m_e^*.

Similarly, the holes created by these electrons in the valence band also behave like a free particle with an effective mass m_h^*. Hence, the electrons in the conduction band and holes in the valence band both contribute to electrical conduction.

Extrinsic semiconductor:- Extrinsic semiconductor is an impure s.c formed from an intrinsic s.c by adding a small quantity of impurity atoms also called dopants.

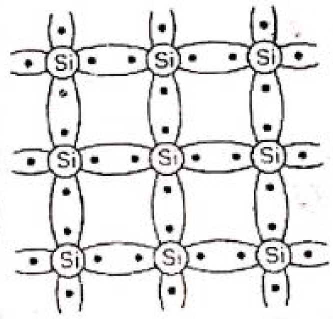
The process of adding impurities to the s.c. crystal is known as doping.

8 Based on the element of doping, the extrinsic s.c. are of two types.

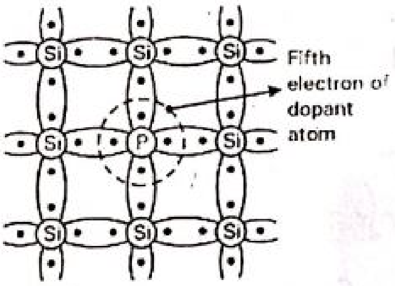
(i) n- type s.c

(ii) p- type s.c.

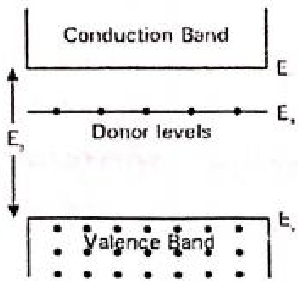
n-type Semiconductor:- A n-type semiconductor gets formed on doping atoms that have five valence electrons to an intrinsic semiconductor like Si or Ge. Consider the intrinsic semiconductor Si which has 4 valence electrons. Each of the four valence electron is covalently bonded with one of the four adjacent Si atoms as shown in fig 1.



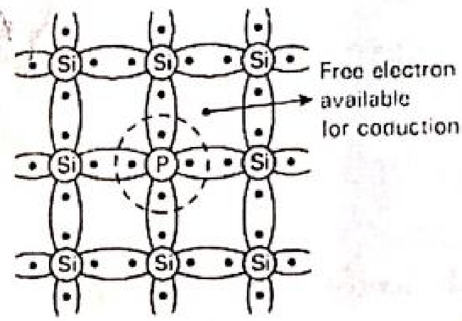
To this Si atom, if an atom with five valence electrons such as phosphorous (P), Arsenic (As) is incorporated into the crystal then of the electrons from the dopant atom will participate in the covalant bond formation there by leaving an extra electron in the unbounded state as shown in fig 2.



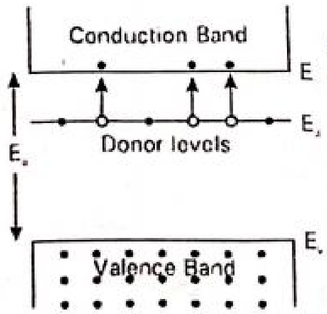
At T = OK



At T-OK



At T > OK



At T > OK

This extra electron is only weakly bound to the atom and enters into an energy level in a donor state just below the conduction band as shown in figure.

Since this extra electron is not tightly bound to the atom, all such electrons at room temperature can get excited to the conduction band even for a small increase in the external energy leaving the parent atom positively ionised.

Since the pentavalent atoms donates electrons to the conduction band in obtaining n-type s.c., they are also called as donor atoms.

Ed (donor energy) is the minimum energy required for the electron to enter the conduction band.

Since excitation of these weakly bound electrons does not result in the formation of a hole, the no. of electrons in such a material far exceeds the no. of thermally generated holes. Hence, in this type of semiconductors, electrons are the majority carriers and the holes are the minority carriers.

In case, If the thermal energy is sufficiently high, in addition to the ionization of donor impurity atoms breaking of covalent bond may also occur thereby giving rise to generation of electron hole pairs.

p-type semiconductor:-

A p-type semiconductor gets formed on doping atoms that have three valence electrons to an intrinsic semiconductor like Si or Ge.

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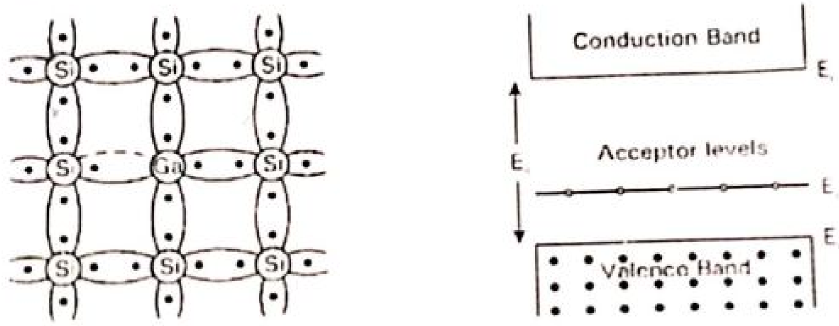
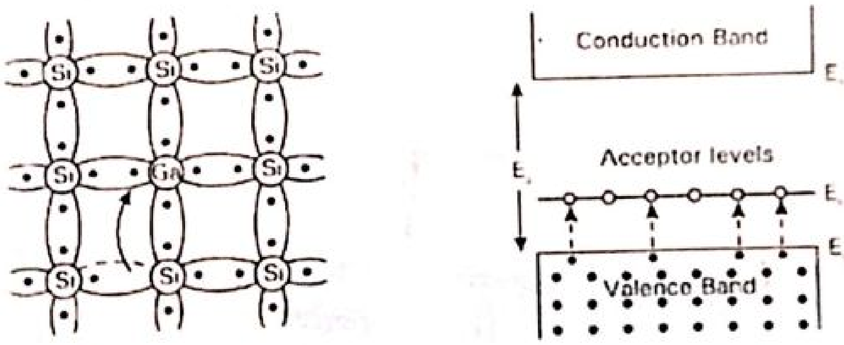
The trivalent elements like Gallium (Ga), Indium (In) or Boron (B) can be added as a dopant to an intrinsic S.C.

Let us assume a trivalent element Ga is added to an intrinsic S.C Si. All the three valence electrons of Ga will form three covalent bonds with three neighbouring Si atoms as shown in figure.



(a) At T = 0K (a) At T = 0K

Figure 11.3 : Charge carrier excitation in a p-type semiconductor



(a) At T > 0K (b) At T > 0K

Thus, the dopant is in need of an extra electron to complete its fourth covalent bond formation with Si.

This extra electron may be supplied by Si, there by creating an electron hole in the valence band that can be filled by electrons from the other locations in the band in turn creating an another vacant site. Thus, the holes act as acceptors of electrons. These hole sites have an energy slightly higher than the normal energy and create an energy level called <u>acceptor energy level</u> which lies just above the valence band.

Since the dopant atoms Ga accepts electrons, they are also called as <u>acceptors</u>.

An electron must gain energy of the order of Ea inorder to create a hole in the valence band. Thus, these acceptor atoms get negatively ionised after accepting the electrons from the valence band even at room temperature. Hence, holes are created in the valence band and are ready for conduction.

when a sufficiently large no. of acceptor atoms are added, the holes greatly out number the thermally excited electrons. Hence, the holes are the majority carriers while electrons are the minority carriers in p-type semiconductor.

In case, if the temperature is sufficiently high, in addition to the above process, additional electron hole pairs also get generated due to breaking of covalent bonds.

NON-EQUILIBRIUM SITUATION :- (EXCESS CARRIERS) :-

In the case of the semiconductor in thermal equilibrium the product of electron and hole concentration is a constant ($n \times p = n_i^2$) for a particular material at a given temperature. However, if excess carriers are introduced in a s.c. so that $np > n_i^2$, a non equilibrium situation arises.

Excess carriers can be introduced in a s.c. by shining light (optical excitation) or forward biasing a p-n junction. This process of introducing excess carriers is called injection. In case of optical excitation, photons are absorbed in s.c. resulting in excitation of electrons from the valence band to conduction band. Thus, the optical excitation results in additional EHPs (electron hole pairs) being generated and a new steady state is achieved where the total generation recombination rate is equal to the total generation rate.

The electron and hole concentrations in this steady state are more than their equilibrium values. These additional carriers are called excess carriers. The magnitude of the excess carriers relative to the equilibrium majority carrier concentration determines the level of injection.

For example, let us consider an n-type silicon sample with $N_D = 10^{15}$ cm^{-3} at 300K. The majority carrier concentration at thermal equilibrium is $n_{no} = 10^{15}$ cm^{-3} and the minority carrier concentration is $p_{no} = 2.25 \times 10^5$ cm^{-3}. Now, let us suppose that by optical excitation

10^{12} excess minority carriers per cm^3 are injected in this sample. The excess electron concentration n_n' must be equal to the excess hole concentration p_n' since excess hole and electron are generated in pairs. Thus, while the minority carrier concentration in sample has increased by nearly seven orders of magnitude (from $2.25 \times 10^5\ cm^{-3}$ to $10^{12}\ cm^{-3}$), the increase in the electron concentration is negligible. This condition where the excess carrier concentration is small compared to the majority carrier concentration i.e

$$n_n' = p_n' << n_{no}$$ is refered to as <u>low level injection</u>

The other case where, $n_n' = p_n' \geq n_{no}$ is called <u>high level injection</u>.