

Element of Material Science

Bonding in Solids $\Rightarrow$

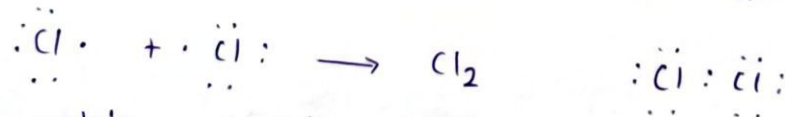
There are various types of bonds existing between atoms constituting a solid. These are produced by the forces between the atoms, ions & molecules.

There are 5 types of bonds :-

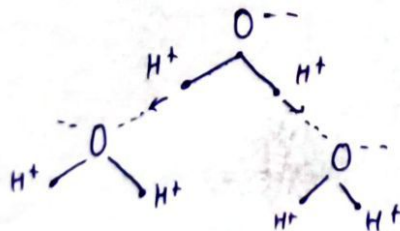
1. Ionic Bond (NaCl, CsCl, MgO)
2. Covalent Bond (C, Si, Ge)
3. Metallic Bond (Na, Al, Cu, Ag, Zn)
4. Hydrogen Bond (H_2O , HF)
5. Vander Waals Bond

1. Ionic Bond :- In an ionic bond b/w two atoms one or more electrons are transferred from one atom to the other with result that one of the atoms becomes positively charged ion & the other negatively charged ion. Eg - NaCl, CsCl, MgO

2. Covalent Bond :- The covalent bond which is sometimes referred to as valence bond or homopolar bond, is an electron-pair in which two atoms share two electrons.
Eg -



3. Hydrogen Bond :- In certain crystals, a positive hydrogen ion (H^+) ~~attaches~~ attracts negative ions such as F^- , O^- , N^- etc. sometimes due to electrostatic attraction, attachment b/w atoms in different molecules.

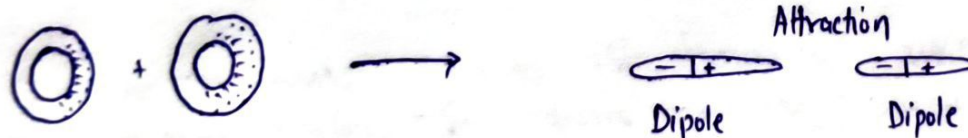


4. Metallic Bond : - Metallic crystals are commonly known as metals. In the atoms of metals, the electrons in the outermost orbits are loosely bound as the Ionization energy is low in case of metals. These electrons are free to move around among all the atoms & are called free electrons or conduction electrons. This way the metals have residual positive ions. The electrostatic attraction b/w these positive ions & negative electrons is responsible for holding the solid together. This type of bonding is called metallic bonding.

5. Vander Waal Bonds or Molecular Bond : -

Many solids or crystals are composed of neutral atoms or molecules without any transferring or sharing of electrons. Hence the ionic covalent & metallic bonds are not possible b/w these atoms. These substances remain bound by much weaker short range attractive forces, which are called Vander Waal Bonds.

These bonds are formed due to electrostatic attraction b/w oscillating or permanent dipoles.

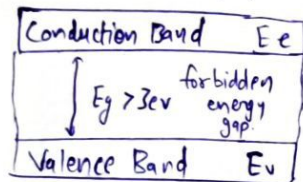


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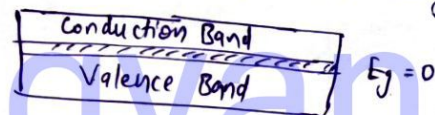
Classification of Solids on basis of Energy Band Gap:-

On the basis of energy band structure & electrical conductivity the solids can be divided into three types:

1. Insulators → For these types of solids, the band formation is like the forbidden gap is very wide, it is about 3eV to 6eV. It is seen that a very few electrons from the filled band reach the empty band. The conductivity is very small of the order of 10^{-12} to 10^{-18} mho/m.



2. Conductor → In this kind of solids the valence & conduction bands are overlapped. Thus in these materials the forbidden energy gap is not present i.e. $\Delta E_g = 0$. Metals like silver copper etc. The conductivity is of the order of 10^6 to 10^8 mho/m.



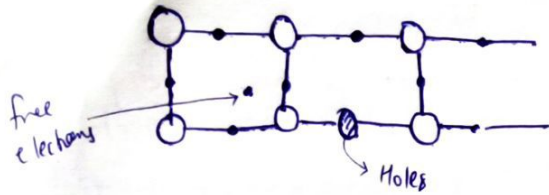
3. Semi conductor :- For this type of solids the forbidden gap is very narrow of about 0.1eV to 1eV. Under this situation electrons can move easily from the highest filled band to next empty band when applied external energy.

(a) Intrinsic

(b) Extrinsic

→ For this reason, a free electron current can be obtained as a few electrons are available in the empty band. This class of solids is known as semi-conductors.

Intrinsic Semiconductors $\Rightarrow$ The transformation of electrons to conduction band & the generation of holes in the valence band are achieved by thermal excitation. It means this effect is temp dependent & produces equal numbers of electron & hole carriers.



Conductivity in Intrinsic Semiconductors $\Rightarrow$

At absolute zero temp. all the valence electrons remain tightly bound in covalent bonds so that there is no electron in conduction band & the conductivity of material is zero. Thus all semiconductors at absolute zero behave as insulators.

If in an intrinsic semiconductor the no. of free electrons & holes per unit volume are n_i & p_i then

$$n_i = p_i$$

$$\Rightarrow n_i \times p_i = n_i^2 \quad \text{--- (1)}$$

Where

A is

constant,

k is Boltzmann Constant.

It decreases exponentially with increase of forbidden energy gap.

$$n_i = AT^{3/2} \exp\left(\frac{-E_g}{2kT}\right) \quad \text{--- (2)}$$

$$v_e = \mu_e E \quad \text{--- (1)}$$

(drift velocity of electrons)

$$v_h = \mu_h E \quad \text{--- (2)}$$

(drift velocity of holes)

Here μ_e = Mobility of electrons

$$J = J_e + J_h \quad \text{--- (3)}$$

$$J = eE(\mu_e n + \mu_h p) \quad \checkmark$$

and conductivity
and Resistivity

μ_h = Mobility of holes

$$\text{But } J_e = n(-e)(-v_e) = \mu_e n E, \quad J_h = p(+e)(+v_h) = \mu_h p E$$

$$\sigma = \frac{J}{E} = e(\mu_e n + \mu_h p) = e(\mu_e n + \mu_h p) \quad \checkmark$$

$$\rho = \frac{1}{\sigma} = \frac{1}{e(\mu_e n + \mu_h p)} \quad \checkmark$$

Extrinsic Semiconductors : As we know conductivity of intrinsic semiconductors are very low. To enhance the conductivity intrinsic semiconductors are doped with a controlled amount of an impurity elements. The obtained semiconductors are so called as Extrinsic Semiconductors.

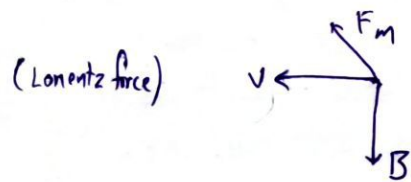
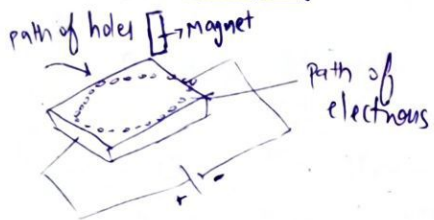
There are two types of Extrinsic semiconductors :-

1. N-type Semiconductor $\Rightarrow$ If an element of 5th group (P, As, Sb) is added to pure semiconductor, the obtained semiconductor is called as N-type semiconductor.

These impurities are known as Dopant. In doping process these dopants replace an atom of intrinsic semiconductor and 4 out of 5 electrons form covalent bonds but one electron remains free. At room temp. this free electron is transferred to conduction band. Since there are negatively charged carriers are taking part in flow of current so the extrinsic semiconductor is called as N-type semiconductor.

2. P-type Semiconductors $\Rightarrow$ When an element of 3rd group (B, In, Ga) is added as impurity in pure semiconductor, the obtained semiconductor is called P-type semiconductor. Since 3rd group elements are trivalent. The energy level of the hole produced by the addition of 3rd group impurities lies in forbidden energy gap slightly above the valence band. As the electrical conduction now is mainly by the holes which behave as positive charged carriers, the doped semiconductor is called P-type Semiconductors.

Hall Effect :- When a magnetic field is applied perpendicular to a current carrying conductor or semiconductor, a voltage is developed across the specimen in a direction perpendicular to both the current & the magnetic field. This phenomenon is called HALL EFFECT & the voltage so developed is called Hall voltage.



A steady state will be achieved when the force due to magnetic field will be balanced by the force due to transverse electric field. In steady state

$q(\vec{v} \times \vec{B}) = -q\vec{E}_t \quad (\text{For Electrons})$ $\vec{E}_t = -(\vec{v} \times \vec{B})$ $\vec{E}_t = -vB(-\hat{x} \times \hat{z})$ $\vec{E}_t = vB(+\hat{y})$	$q(-\vec{v} \times \vec{B}) = q\vec{E}_t \quad (\text{For Holes})$ $\vec{E}_t = -(\vec{v} \times \vec{B})$ $\vec{E}_t = -vB(-\hat{x} \times \hat{z})$ $\vec{E}_t = vB(+\hat{y})$
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Hall Coefficient :- The average drift velocity $\vec{v}$ is related to current density $\vec{J}$ as

$$\vec{J} = nq\vec{v}$$

$$v = \frac{1}{nq}$$

Since $E_t = vB$

$$\therefore E_t = \frac{1}{nq}(B) = \frac{1}{nq}(JB)$$

* If thickness of semiconductor bar is 'd'

then $E_t = \frac{V_h}{d}$

$$\frac{V_h}{d} = \frac{1}{nq}(JB)$$

$$\text{or } \boxed{V_h = \frac{d}{nq}(JB)}$$

Hall Voltage

$$\boxed{\frac{1}{nq} = R_h}$$

Hall Coefficient

Fermi Energy $\Rightarrow$

It is a concept of quantum mechanics usually referring to the energy difference b/w highest & lowest occupied single particle states in quantum system of non-interacting fermions at absolute zero temperature.

$\Rightarrow$ At $T > 0K$

$$f(E) = \frac{1}{2}, \quad f(E_F) = \frac{1}{2} = 0.5$$

[At $0K$ temp, highest energy of outermost shell (valence band) is defined as fermi energy]

$\rightarrow$ In a system of fermions, such as electrons in a metal, the energy separating the highest occupied single-particle state from lowest occupied one.

$\rightarrow$ The highest filled energy level at absolutely zero for a fermion is called the fermi level. All energy levels below this value are occupied, & all above this value are empty.

Fermi - Function $\Rightarrow$

The distribution of electrons in beta decay is calculated from the weak interaction

transition matrix using plane wave functions for electrons. However, electron experience the Coulomb field of nucleus, so correct distribution must be modified by fermi-function, which accounts for this effect.

$$f(E) =$$

$$\frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$

$\Rightarrow$ At $T = 0K$

for

$$E < E_F$$

$$f(E) = 1$$

& $E_F = \text{Fermi energy}$
 $k = \text{Boltzmann constant}$

$$E > E_F$$

$$f(E) = 0$$

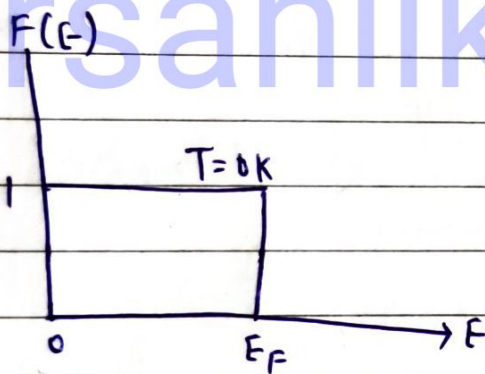
When T is kT then

$$E = E_F - kT$$

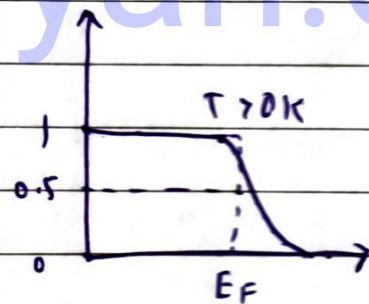
$$F(E) = \frac{1}{e^{1} + 1} = 0.73 = 73\%$$

When $E = E_F + kT$

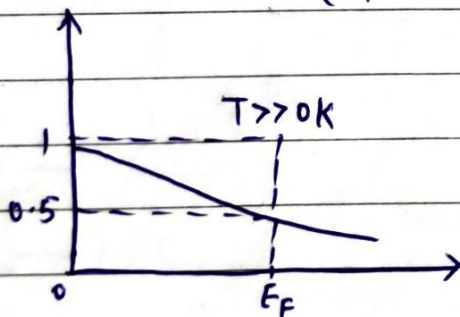
$$F(E) = \frac{1}{e^{(1)} + 1} = 0.27 = 27\%$$



(a)



(b)



(c)

(a) $T = 0\text{ K}$

(b) $T > 0\text{ K}$

(c) $T \gg 0\text{ K}$