Lecture (3)

Band Theory of Solids

- A quantum-mechanical theory of the motion of electrons in solids which predicts certain restricted ranges, or bands, for the electron energies.
- If the atoms of a solid are separated from each other to such a distance that they do not interact, the energy levels of the electrons will then be those characteristic of the individual free atoms, and thus many electrons will have the same energy. As the distance between atoms is decreased, the electrons in the outer shells begin to interact, thus altering their energy and broadening the sharp energy level out into a range of possible energy levels called a band. One would expect the process of band formation to be well advanced for the outer, or valence, electrons at the observed interatomic distances in solids. Once the atomic levels have spread into bands, the valence electrons are not confined to individual atoms, but may jump from atom to atom with an ease that increases with the increasing width of the band.
- Under external influences, such as irradiation, electrons can make transitions between states in the same band or in different bands. The interaction between the electrons and the vibrations of the crystal lattice can scatter the electrons in a given band with a substantial change in the electron momentum, but only a slight change in energy. This scattering is one of the principal causes of the electrical resistivity of metals.
- Thus the band theory of solids takes into account the interaction between the electrons and the lattice ions.in crystal atoms interact and bind by sharing valance electrons.one effect of the interaction between the atoms is that the otherwise degenerate energy levels split into closely spaced levels. since the number of atoms is large (N) , it is common to refer to this set off levels closely packed discrete energy levels, the bands become essentially continuous energy band.
- In solid material there usually exist a valance band (have the highest filled energy and is at the greatest distance from the nucleus also the electrons with lower energy levels are described as occupying the valence band) The top of the valence band for a material is the highest level, which would, in theory, be filled by all the available electrons within an atom of that material at a temperature of 0 K.. and conduction band is defined to be the lowest unfilled energy band, also the space between the valance band and conduction bend is called forbidden energy gap (Eg) as shown in fig.(1)

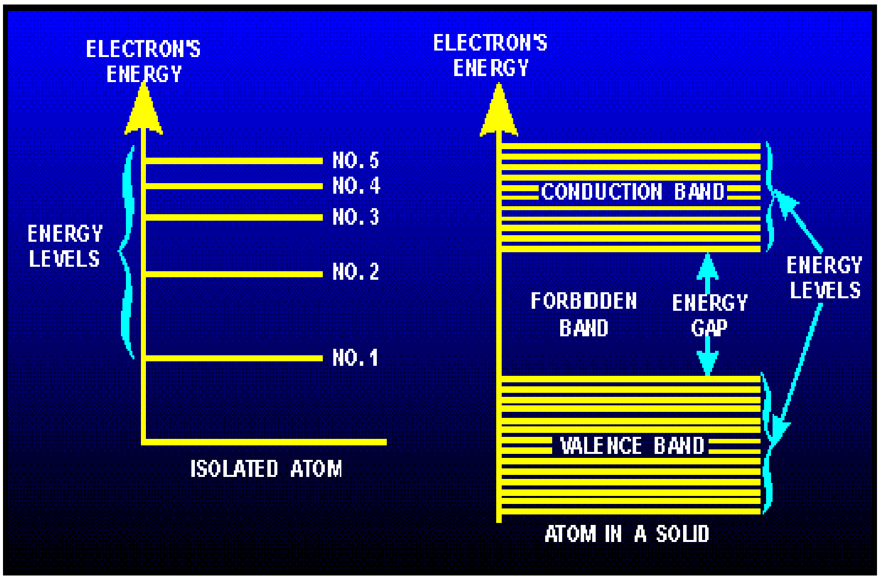
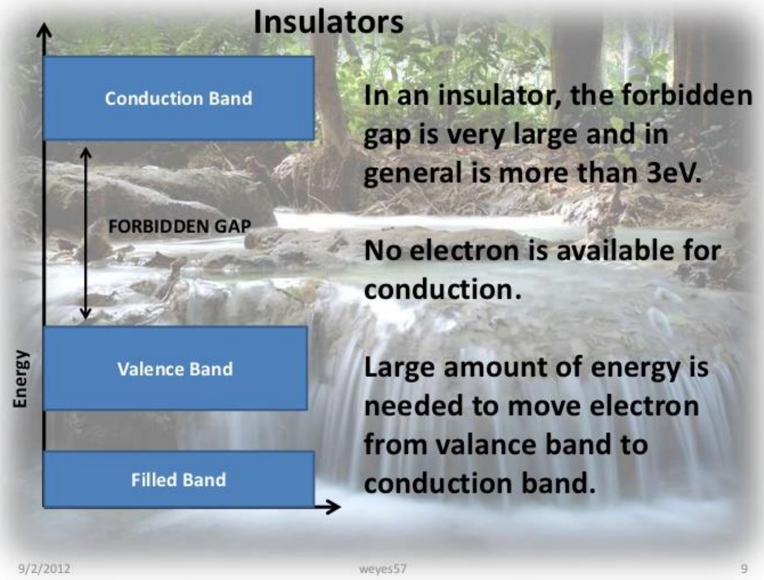


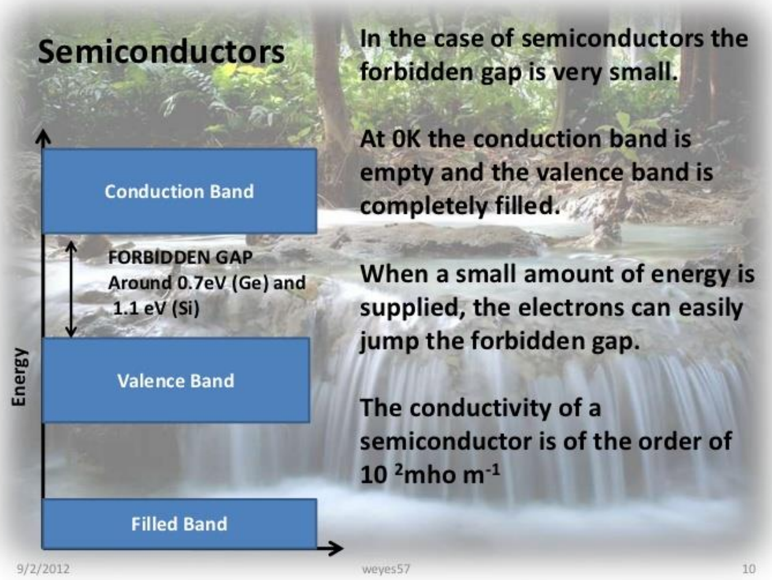
Fig. (1)

show the type of bands

All solids can be classified as conductors, semiconductors and insulators according to the availability of conduction electrons in their structures. Band theory gives an explanation for these differences in electrical properties and accounts for the availability, or not, of those conduction electrons.



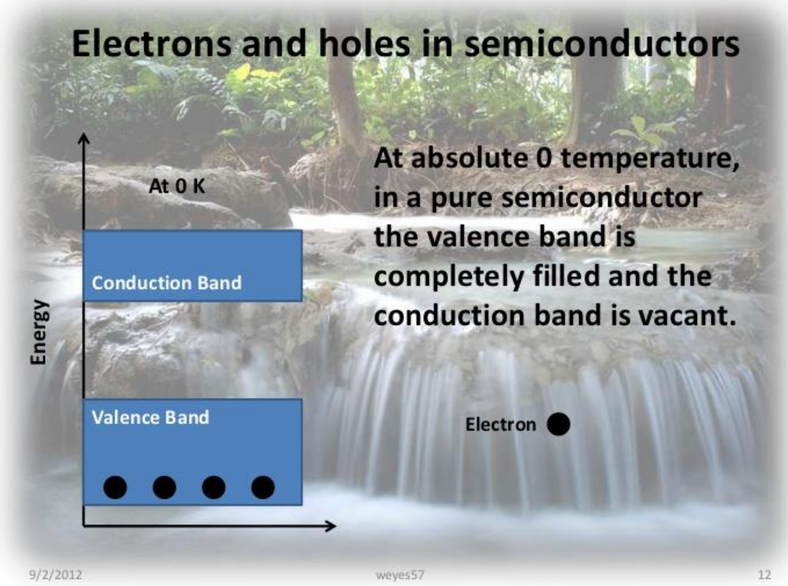
In insulators this zone of forbidden energy levels is very substantial, and separates the valence band and the conduction band significantly. The forbidden zone is of the order of a few electron volts, and is therefore so large that it is not normally practicable for there to be sufficient energy to move electrons across it from the valence band to the conduction band. Contrastingly, conductors only have one band, and the top of this band is only partially filled, permitting electrical conduction. This means that there are plenty of nearby energy levels available for electrons to move into. They can flow easily from one atom to another when a potential difference is applied across the conducting material.



Like insulators, semiconductors have a completely full valence band and so electrons are not able to facilitate conduction at low temperatures. However, for semiconductors, the forbidden energy level zone between the two bands is sufficiently small to make it much easier for significant numbers of electrons to move across this gap and go from the valence band to the conduction band. This can happen if sufficient energy is supplied, for example if there is some thermal excitation. As a result, semiconductors exhibit increased conductivity with increasing temperatures. In many semiconductors, a temperature increase of 10 K will permit a doubling of the numbers of electrons in the conduction band.

Transport in Semiconductor

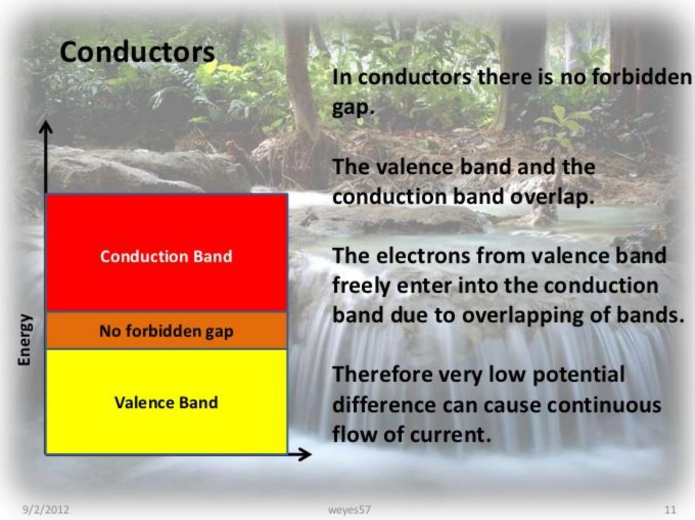
At low temperature , little thermal energy is available to push valance electron across this gap, and the semiconductor material act s more as an insulator. At higher temperatures thought the ambient thermal energy becomes enough to force electrons across the gap , and the material will increase conduction of electricity.



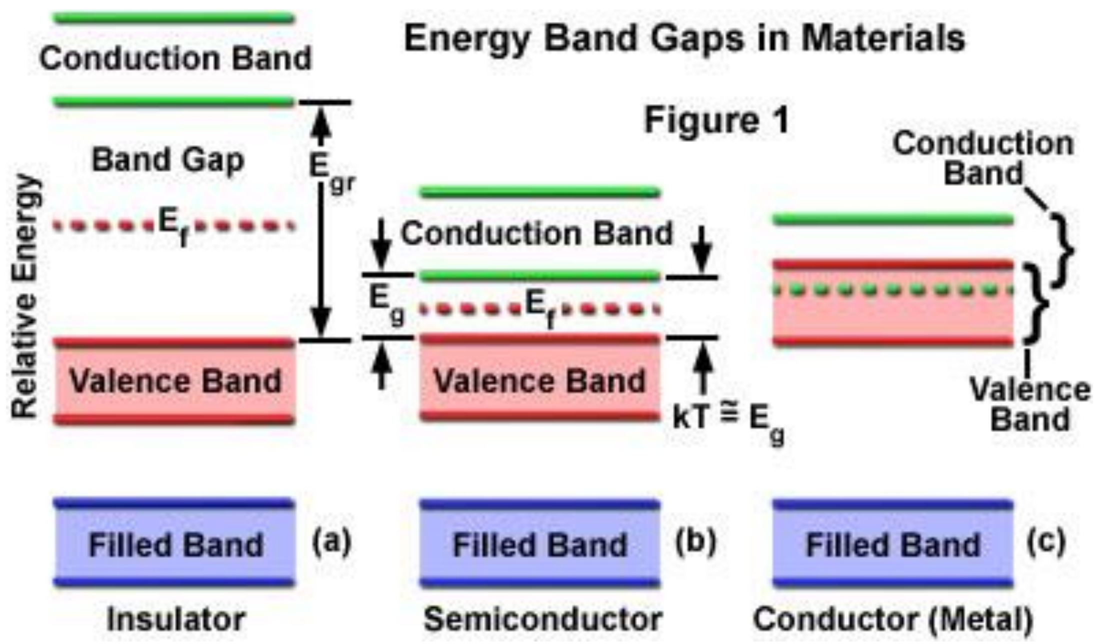
Also in order to increase the conductivity of semiconductors, small amounts of doping material can be used. This results in significant increases in conductivity as a result of the narrowing of the gap between the conduction and valence bands.

Under these external effects the electrons that get excited into conduction band carry current, the space left behind in the valance band is called a hole. Holes also conduct current and they have positive charge .

conductors have the conduction and valance band overlapping and Fermi level falls inside the energy band ,easy electron to move .



The below figure shows the differ between three types of solid according the differences of bands



Summary of band theory

- In solids, permitted electron energy levels are organized as bands, The essential feature of the band theory is that the allowed energy states for electrons are nearly continuous over certain ranges, called **energy bands.**
- The **valence band** contains electrons that can be considered to be bound to the atom. In insulators and semiconductors the valence band is full.
- The **conduction band** is a region of permitted energy levels that is empty in insulators and semiconductors, but partially filled in conductors.
- E_g it is a forbidden zone that forms an **energy gap** between the valence and conduction bands in insulators and semiconductors
- The band structures of insulators and semiconductors resemble each other qualitatively. Normally there exists in both insulators and semiconductors a filled energy band (referred to as the **valence band**) separated from the next higher band (referred to as the **conduction band**) by an energy gap.
- If this gap is at least several electron volts, the material is an **insulator.** It is too difficult for an applied field to overcome that large an energy gap, and thermal excitations lack the energy to promote sufficient numbers of electrons to the **conduction band.**
- When the temperature is increased from $T = 0$, more and more atoms are found in excited states. The increased number of electrons in excited states explains the temperature dependence of the resistivity of semiconductors.
- **Doping** of semiconductors can significantly reduce the width of the energy gap. Only those electrons that have jumped from the **valence band** to the **conduction band** are available to participate in the conduction process in a semiconductor.

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Ionic, Covalent and Metallic Bonding: -

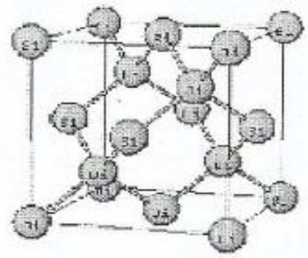
Most of material is either solids or liquid which hold together by inters atomic forces. inter atomic forces are caused by electrons in the shells of the atoms forming the solid, Nobel gases have a completely full shell this resulting in the stable elements which have very little attraction to each other because of this stable electron cloud. most other elements do not have this stable arrangement. These electrons attempt to reach this stable state by one of three types mechanism and in the development of electronic materials. these materials must in addition crystal line structure in their atomic arrangment,it is this periodic crystalline structure that provides most of the properties of interest in electronic.

· Crystalline solid may be define A volume of atoms covalently bonded in a periodic structure with Well-defined symmetries.

–Example: Silicon

• Face-Centered Cubic (FCC) structure

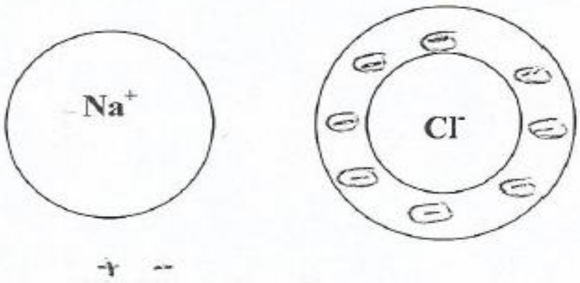
• Group-IV elements (4 valence electrons)



In considering the origin of this crystalline structure, we begin by studying the nature of atomic bonding.

1-Ionic Bonding: -

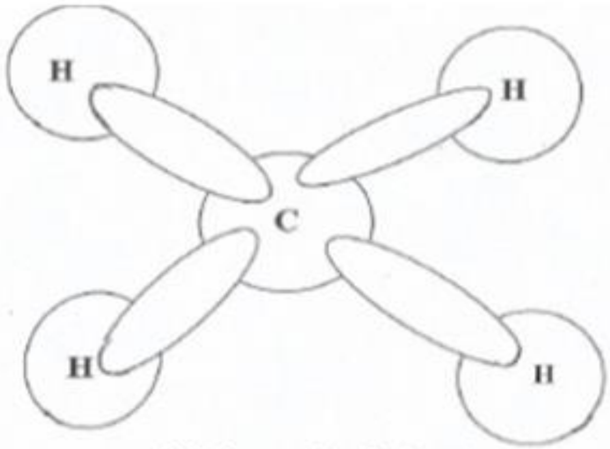
The ionic bonding, formed when one of he atomic constituents yields an outer-shell electron to the other atom, producing a set of positive and negative ions which attract by means of a coulomb-type attraction .for example in (NaCl) in which a single electron is transferred. this bond is a strong bond and non directional.



NaCl molecular

2-Covalent bonding:-

In covalent bonding, the electrons are shared between two or more neighboring atoms. Elements from the central group (4) are not readily ionized. The energy required to remove all the valance electrons are too large for ionic bonding to be possiple.it is possible for each atom to complete its outer-shell, by sharing electrons with its neighbours.such carbon has atomic number (6) that has four electrons in the second shell which required to gain more electrons to be completely full (CH_4). The molecules themselves are not attracted to each other.



Methane cloud structure

3-Metallic Bonding:-

This type of bonding is very similar to covalent bonding, except that many atoms share the valance electrons. The majority of elements are metals, which have small number of valance electron in the outer shell these electrons called "Free electrons". In the metal atom the outer electronic shell is only partially filled, usually by no more than 3-electrons.

Copper for example .in the solid copper all the valance electrons can move about freely between the copper ions alattice of positive ions embedded in a sea of electrons.

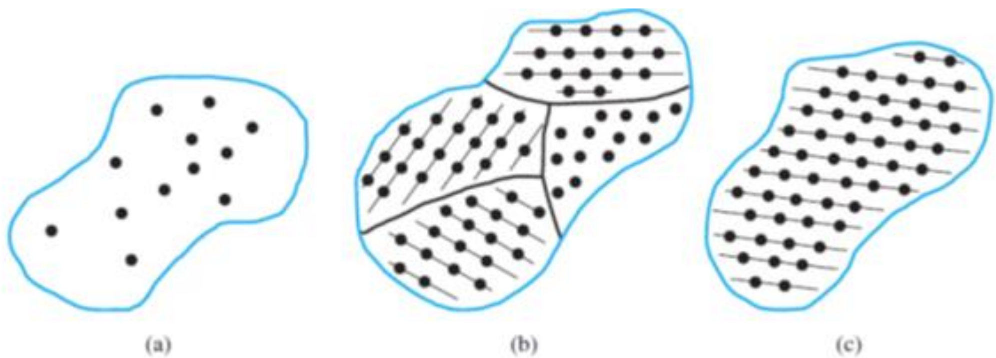
TYPES OF SOLIDS

Amorphous, polycrystalline, and single crystals are the three general types of solids. Each type is characterized by the size of an ordered region within the material as shown in below figure .

a- a amorphous materials have an ordered region is a spatial volume in which atoms or molecules have a regular geometric arrangement or periodicity. Amorphous materials have order only within a few atomic or molecular dimensions.

b- polycrystalline materials have a high degree of order over many atomic or molecular dimensions. These ordered regions, or single-crystal regions, vary in size and orientation with respect to one another.

c- The single-crystal regions are called grains and are separated from one another by grain boundaries. Single-crystal materials, ideally, have a high degree of order, or regular geometric periodicity, throughout the entire volume of the material. The advantage of a single-crystal material is that, in general, its electrical properties are superior.



Schematics of three general types of crystals : a) amorphous, b) polycrystalline , c) single crystal