Chapter 4

Modern Physics

1- The solid state and crystal structure:

Matter exists in three distinct states:

1- Gase state: where,

a) Molecules are in continuous motion; translational, rotational and vibrational.

b) These particles are very small compared with the volume of the space they occupy.

c) They exert little or no force upon one another.

d) Fill all the space they occupy.

e) The particles strike the walls of the container thus constituting the pressure of the gas.

2- Liquid state: where,

a) The particles become much closer to each other.

b) Take the shape of any container in which they are placed.

c) The motion of molecules is in random and them relative position change continuously.

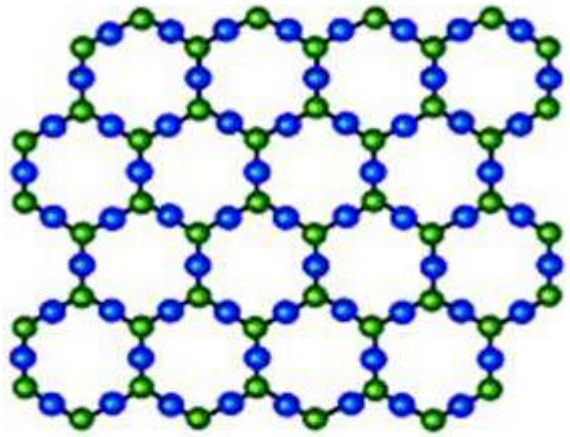
3- Solid state: where,

a) The translational motion of atoms becomes very small and vanishing.

b) The position of every atom relative to its neighbours is fixed.

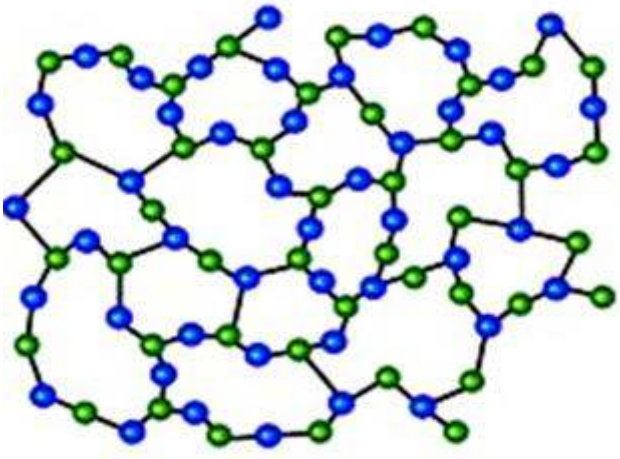
c) Has a certain volume and shape.

d) Solids can be classified into two types:



1- Crystalline materials:

Where, atoms are distributed in an orderly manner. Atoms (ions or molecules) in repeating 3D pattern (called a lattice).



2- Amorphous materials:

Where, the internal structure is not distributed in an orderly manner. Short range order, not periodic; ex: glass.

Bonding in Solids

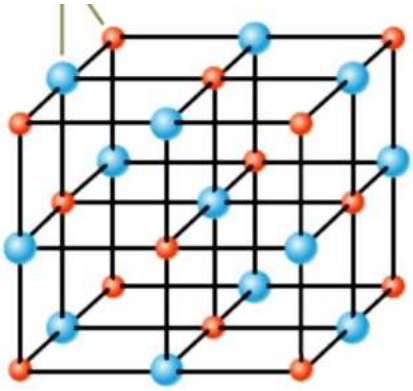
A crystalline solid consists of a large number of atoms arranged in a regular array, forming a periodic structure. These atoms are held in their positions by forces called bonds. Bonding forces differ in nature and strength from one crystal to another as:

Ionic Solids:

Many crystals are formed by ionic bonding, in which the dominant interaction between ions is the Coulomb force. For example, sodium chloride crystal Na^+ Cl^- where, the sodium atom has one electron in its outer most orbit. So, when this electron is removed the sodium ion attains an electronic configuration similar to the nearest inert gas which is more stable. On the other hand, the chlorine atom has seven electrons in its outer most orbit. So, when it receives an electron, its configuration attains an electronic configuration similar to the nearest inert gas which is more stable also.

So, the ions of each sodium and chlorine arrange themselves so as to maintain electrical neutrality inside the crystal.

Consider a portion of the NaCl crystal shown in the opposite figure. The larger spheres are sodium ions, and the smaller spheres are chlorine ions. Each Na^+ ion has six nearest-neighbor Cl^- ions. Similarly, each Cl^- ion has six nearest-neighbor Na^+ ions.



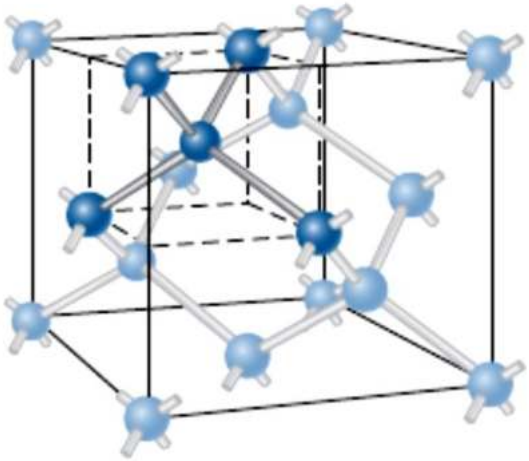
Ionic crystals form relatively **stable, hard crystals**. They are **poor electrical conductors** because **they contain no free electrons**; each electron in the solid is bound tightly to one of the ions, so it is not sufficiently mobile to carry current.

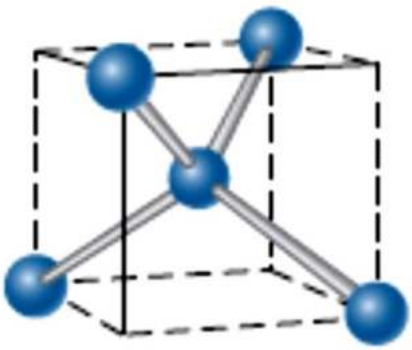
Ionic crystals **have high melting points**; for example, the melting point of NaCl is 801°C.

Ionic crystals are **transparent to visible radiation because the shells formed by the electrons in ionic solids are so tightly bound** that visible radiation does not possess sufficient energy to promote electrons to the next allowed shell.

Covalent Solids

Solid carbon, in the form of diamond, is a crystal whose atoms are covalently bonded. Carbon atom has four electrons in its outer most orbit. So, in the diamond crystalline structure, each carbon atom is covalently bonded to four other carbon atoms located at four corners of a cube as shown in the Figure to can accommodate eight electrons which





The basic structure of diamond is called tetrahedral (each carbon atom is at the center of a regular tetrahedron), and the angle between the bonds is 109.5°. Other crystals such as silicon and germanium have the same structure.

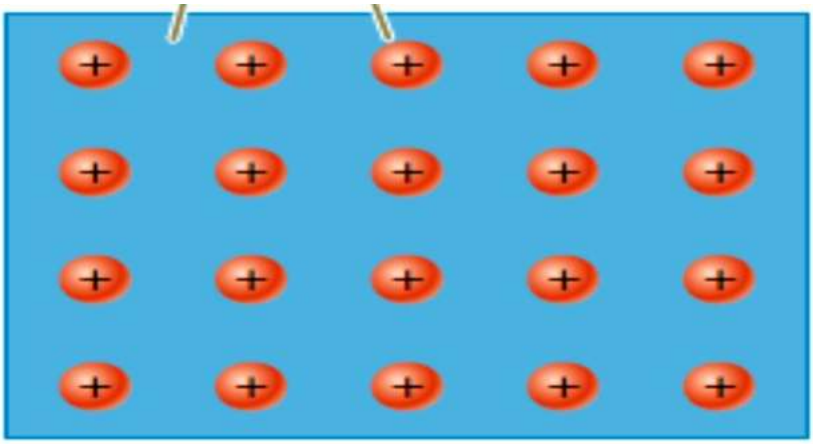
Carbon is interesting in that it can form several different types of structures. In addition to the diamond structure, it forms graphite, with completely different properties. In this form, the carbon atoms form flat layers with hexagonal arrays of atoms. A very weak interaction between the layers allows the layers to be removed easily under friction, as occurs in the graphite used in pencil lead.

The atomic cohesive energies of some covalent solids are given in the following table. The large energies account for the hardness of covalent solids. Diamond is particularly hard and has an extremely high melting point (about 4000 K). **Covalently bonded** solids are usually **very hard**, **have high bond energies** and **high melting points**, and **are good electrical insulators**.

Solid	Cohesive Energy (eV per ion pair)
C (diamond)	7.37
Si	4.63
Ge	3.85
InAs	5.70
SiC	6.15
ZnS	6.32
CuCl	9.24

Metallic Solids

Metallic bonds are **generally weaker than ionic or covalent bonds**. **The outer electrons in the atoms of a metal are relatively free to move throughout the material**, and the number of such mobile electrons in a metal is large. The metallic structure can be viewed as a "sea" or a "gas" of nearly free electrons surrounding a lattice of positive ions.



The bonding mechanism in a metal is the **attractive force between the entire collection of positive ions and the electron gas**. Metals have a cohesive energy in the range of 1 to 3 eV per atom, which is less than the cohesive energies of ionic or covalent solids.

Light interacts strongly with the free electrons in metals. Hence, visible light is absorbed and re-emitted quite close to the surface of a metal, which accounts for the shiny nature of metal surfaces. In addition to the **high electrical conductivity** of metals produced by the free electrons, the nondirectional nature of the metallic bond allows many different types of metal atoms to be dissolved in a host metal in

varying amounts. **The resulting solid solutions, or alloys**, may be designed to have particular properties, such as tensile strength, ductility, electrical and thermal conductivity, and resistance to corrosion.

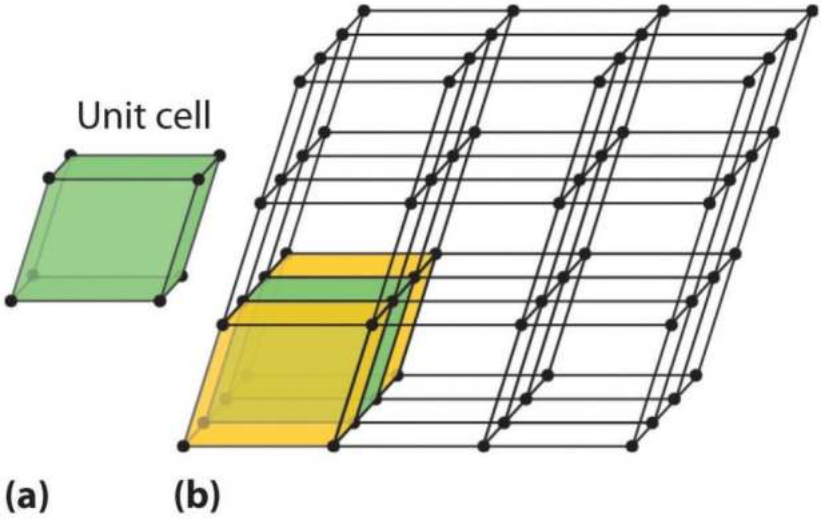
Because the bonding in metals is between all the electrons and all the positive ions, **metals tend to bend when stressed**. This bending is in contrast to nonmetallic solids, which tend to fracture when stressed. Fracturing results because bonding in nonmetallic solids is primarily with nearest-neighbor ions or atoms. When the distortion causes sufficient stress between some set of nearest neighbors, fracture occurs.

crystal structure

To discuss crystalline structures it is useful to consider atoms as being hard spheres with well-defined radii.

The central feature of crystalline structure is that, it is regular and repeating. Any crystalline structure could be described as a pattern formed by repeating various structure units called a **unit cell**.

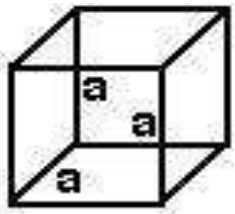
The unit cell can be defined as: **The smallest repeating unit of the lattice.** The length of the unit cell edges and the angles between crystallographic axes are referred to as lattice constants or lattice parameters.



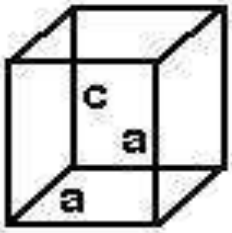
The description of crystal structures by means of unit cells has an important advantage. All possible structures reduce to a small number of basic unit cell geometries. This is demonstrated in two ways:

1- There are only seven unit cell shapes that can be stacked together to fill three dimensional spaces. These are referred to as **the seven crystal systems.**

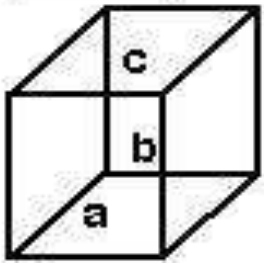
Cubic $a = b = c$, $\alpha = \beta = \gamma = 90^\circ$



Tetragonal $a = b \neq c$, $\alpha = \beta = \gamma = 90^\circ$

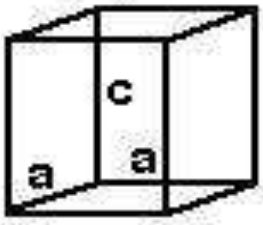


Orthorhombic $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$

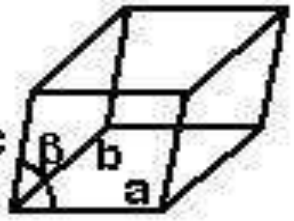


Rhombohedral $a = b = c$, $\alpha = \beta = \gamma \neq 90^\circ$

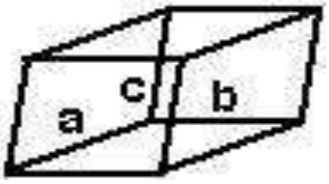
Hexagonal $a = b \neq c$, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$



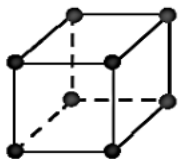
Monoclinic $a \neq b \neq c$, $\alpha = \gamma = 90^\circ \neq \beta$



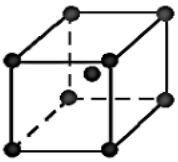
Triclinic $a \neq b \neq c$, $\alpha \neq \beta \neq \gamma \neq 90^\circ$



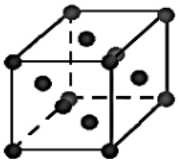
2- There are a limited number of possibilities to show how atoms can be stacked together within a given unit cell. These are referred to as **the fourteen Bravais lattice.**



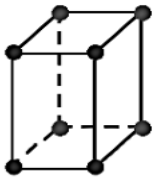
simple cubic



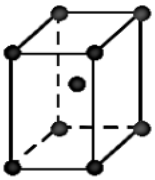
body-centered cubic



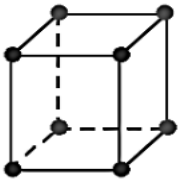
face-centered cubic



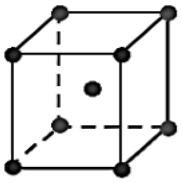
simple tetragonal



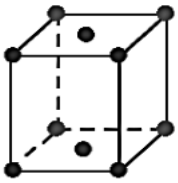
body-centered tetragonal



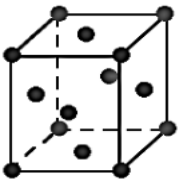
simple orthorhombic



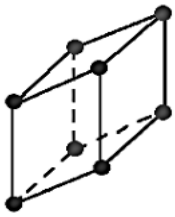
body-centered orthorhombic



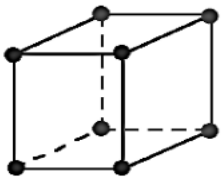
base-centered orthorhombic



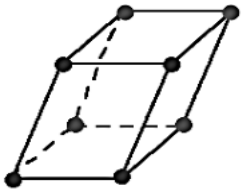
face-centered orthorhombic



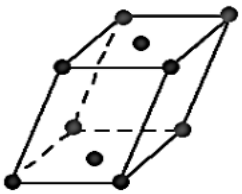
rhombohedral



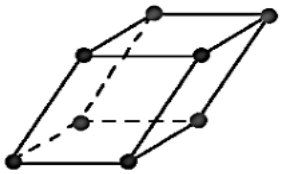
hexagonal



simple monoclinic



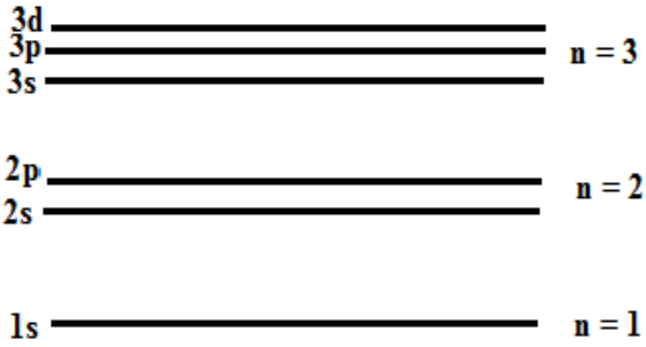
base-centered monoclinic



triclinic

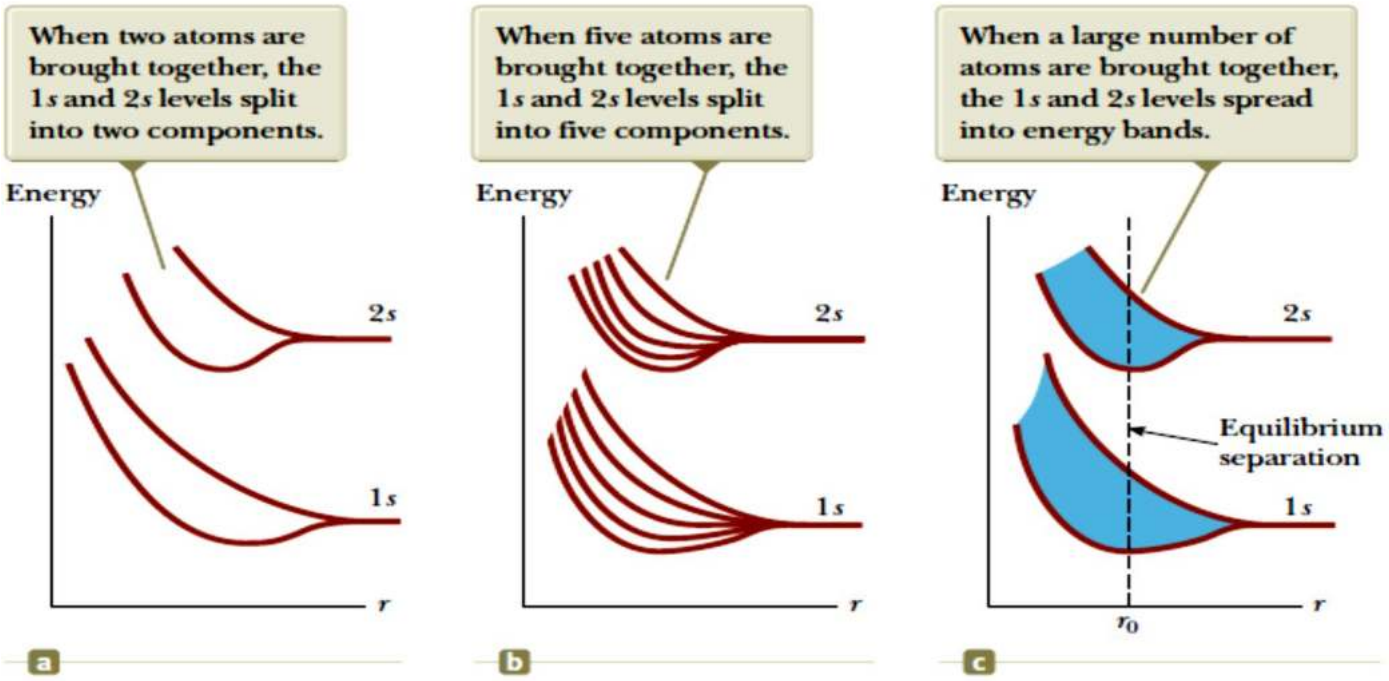
The Band Theory of Solids

From the atomic structure for any single atom, we find that, this atom has principle energy levels donated by the symbol n (K, L, M, N, O, P and Q) which split into sub energy levels donated by the symbol ℓ (s, p, d and f) which split also into orbitals (1 for s, 3 for p, 5 for d and 7 for f) each orbital has two electrons.



So, if two identical atoms are very far apart, they do not interact and their electronic energy levels can be considered to be those of isolated atoms.

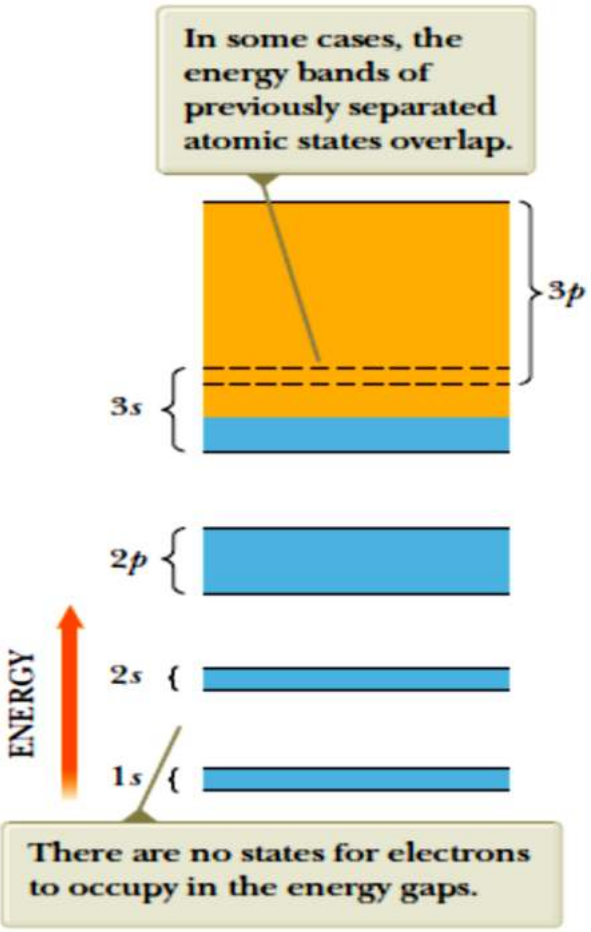
As the two atoms are brought closer so that the distance r between them decreases, the electron cloud of each atom overlap and seems as a splitting of the sub energy level was occurred as seen in Figure a.



When a large number of atoms are brought together to form a solid, a similar phenomenon occurs. As the atoms are brought close together, the various isolated-atom energy levels split into multiple energy levels for the composite system. This splitting in levels for five atoms in close proximity is shown in Figure b. In this case, there are five energy levels corresponding to five different combinations of isolated-atom wave functions.

If we extend this argument to the large number of atoms found in solids (on the order of 10^{23} atoms per cubic centimeter), we obtain a large number of levels of varying energy so closely spaced that they may be regarded as a continuous band of energy levels as shown in Figure c.

The opposite Figure shows the allowed energy bands of sodium, as example, at a fixed separation distance between the atoms. Notice that energy gaps, corresponding to forbidden energies, occur between the allowed bands. In addition, some bands exhibit sufficient spreading in energy that there is an overlap between bands arising from different quantum states (3s and 3p).



The capacity of each band for a system of N atoms is **$2(2\ell + 1)N$** electrons. Therefore, the 1s and 2s bands each contain 2N electrons (ℓ=0), and the 2p band contains 6N electrons (ℓ=1). Because sodium has only one 3s electron and there are a total of N atoms in the solid, the 3s band contains only N electrons and is partially full. The 3p band, which is the higher region of the overlapping bands, is completely empty.

Band theory allows us to build simple models to understand the behavior of conductors, insulators, and semiconductors as well as that of semiconductor devices, as we shall discuss in the following sections.

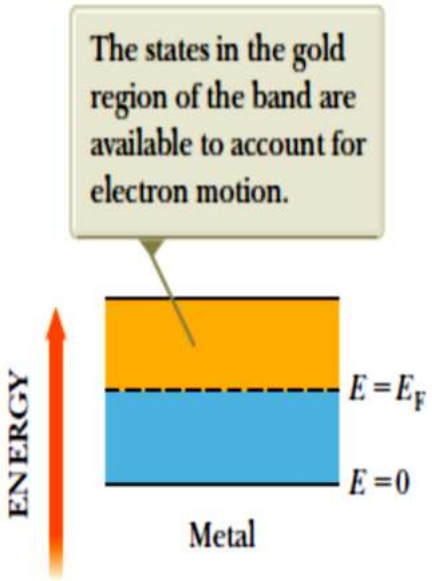
Electrical Conduction in Metals, Insulators, and Semiconductors

Good electrical **conductors contain a high density of free charge carriers,** while in the **insulators**; **the density of free charge carriers is nearly zero**. **Semiconductors,** are a class of technologically important materials in which **charge-carrier densities are intermediate between those of insulators and those of conductors**. In this section, we discuss the mechanisms of conduction in these three classes of materials in terms of a model based on energy bands.

1- Conductors

If a material is to be a good electrical conductor, the charge carriers in the material must be free to move in response to an applied electric field. Let's consider the electrons in a metal as the charge carriers. When an electric field is applied to a conductor, electrons must move upward to an available higher energy state on an energy-level diagram.

The Figure shows a half-filled band in a metal at T = 0 K, where, **The level where all levels below it are filled with electrons and all levels above it are empty**, is called **Fermi energy level**. The Fermi energy lies in the band at the highest the filled state.

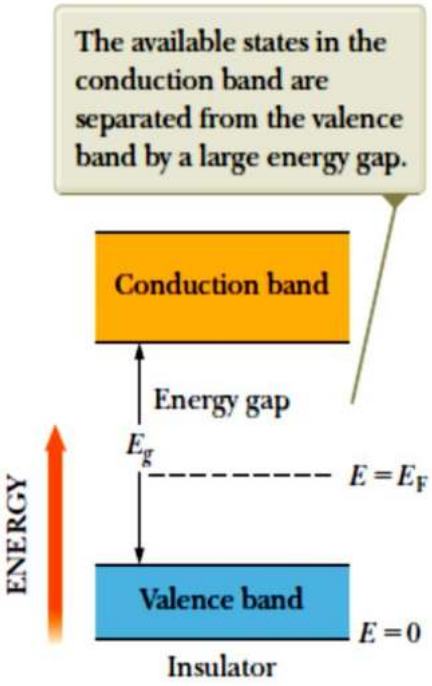


At temperatures slightly greater than 0 K, some electrons are thermally excited to levels above E_F, but overall there is little change from the 0 K case. **If a potential difference is applied to the metal**, however, **electrons** having energies near the Fermi energy **require only a small amount of additional energy** from the applied electric field **to reach nearby empty energy states above the Fermi energy**. **Therefore, electrons in a metal experiencing only a weak applied electric field are free to move because many empty levels are available close to the occupied energy levels.** The model of metals based on band theory demonstrates that metals are excellent electrical conductors.

2- Insulators

Now consider the two outermost energy bands of a material in which the lower band is filled with electrons and the higher band is empty at 0 K. The lower, filled band is called the valence band, and the upper, empty band is the conduction band. (**The conduction band is the band that is partially filled in a metal**, while **the valence band is the band that is completely filled**) It is common to refer to **the energy separation between the valence and conduction bands** as **the energy gap E_g** of the material. Suppose a material has a relatively large energy gap of, for example, approximately 5 eV. At 300 K (room temperature), $k_BT = 0.025$ eV, which is much smaller than the energy gap.

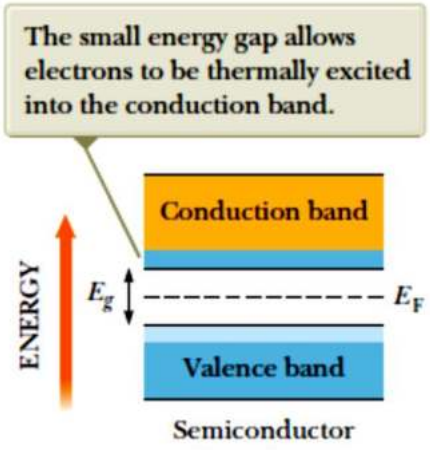
At such temperatures, very few electrons are thermally excited into the conduction band. **There are no available states that lie close in energy above the valence band and into which electrons can move upward to account for the extra kinetic energy associated with motion through the material in response to an electric field. Consequently, the electrons do not move; the material is an insulator.**



Although an insulator has many vacant states in its conduction band that can accept electrons, these states are separated from the filled states by a large energy gap. Only a few electrons occupy these states, so the overall electrical conductivity of insulators is very small.

3- Semiconductors

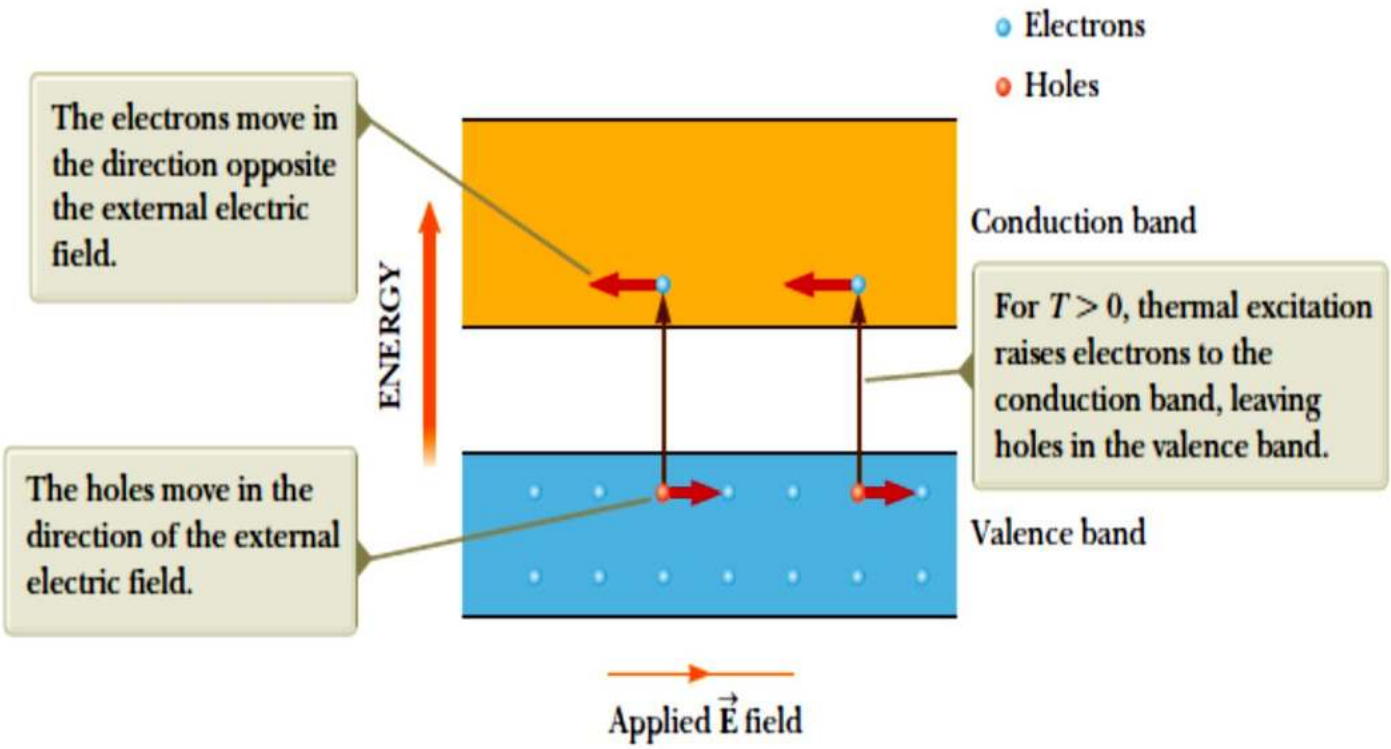
Semiconductors have the same type of band structure as an insulator, but the energy gap is much smaller, on the order of 1 eV. Because the E_g is small, appreciable numbers of electrons are thermally excited from the valence band to the conduction band.



Because of the many empty levels above the thermally filled levels in the conduction band, a small applied potential difference can easily raise the energy of the electrons in the conduction band, resulting in a moderate current. **At T = 0 K, all electrons in these materials are in the valence band and no energy is available to excite them across the energy gap. Therefore, semiconductors are poor conductors at very low temperatures.** Because the thermal excitation of electrons across the narrow gap is more probable at higher temperatures**, the conductivity of semiconductors increases rapidly with temperature, contrasting** sharply with the conductivity of metals, which decreases slowly with increasing temperature.

Charge carriers in a semiconductor can be negative, positive, or both. When an electron moves from the valence band into the conduction band, it leaves behind a vacant site, called a hole, in the otherwise filled valence band. This hole (electron deficient site) acts as a charge carrier in the sense that a free electron from a nearby site can transfer into the hole. Whenever an electron does so, it creates a new hole at the site it abandoned. Therefore, the net effect can be viewed as the hole migrating through the material in the direction opposite the direction of electron movement. The hole behaves as if it were a particle with a positive charge +e. A pure semiconductor crystal containing only one element or one compound is called an intrinsic semiconductor. In these semiconductors, there are equal numbers

of conduction electrons and holes. Such combinations of charges are called electron–hole pairs.

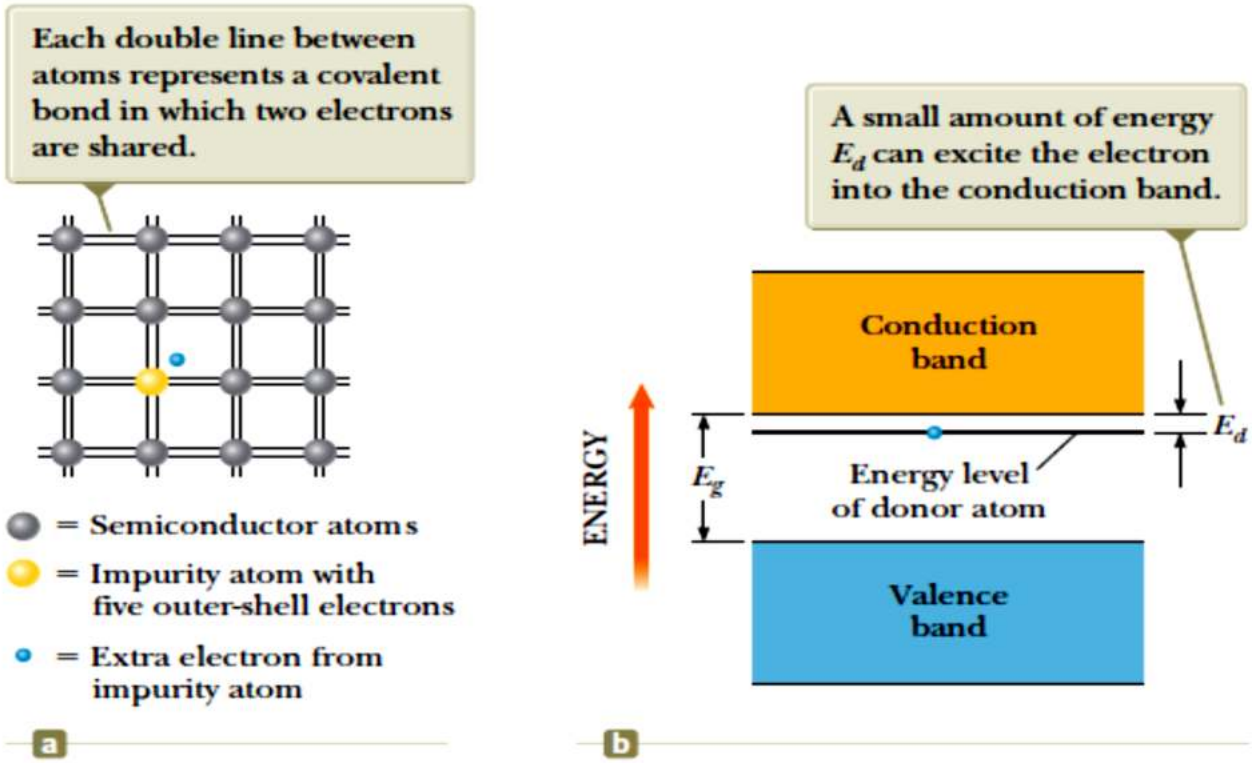


In the presence of an external electric field, the holes move in the direction of the field and the conduction electrons move in the direction opposite the field.

Doped Semiconductors

When impurities are added to a semiconductor, both the band structure of the semiconductor and its resistivity are modified. The process of adding impurities, called doping, is important in controlling the conductivity of semiconductors. For example, when an atom containing five outer-shell electrons, such as arsenic, is added to a Group

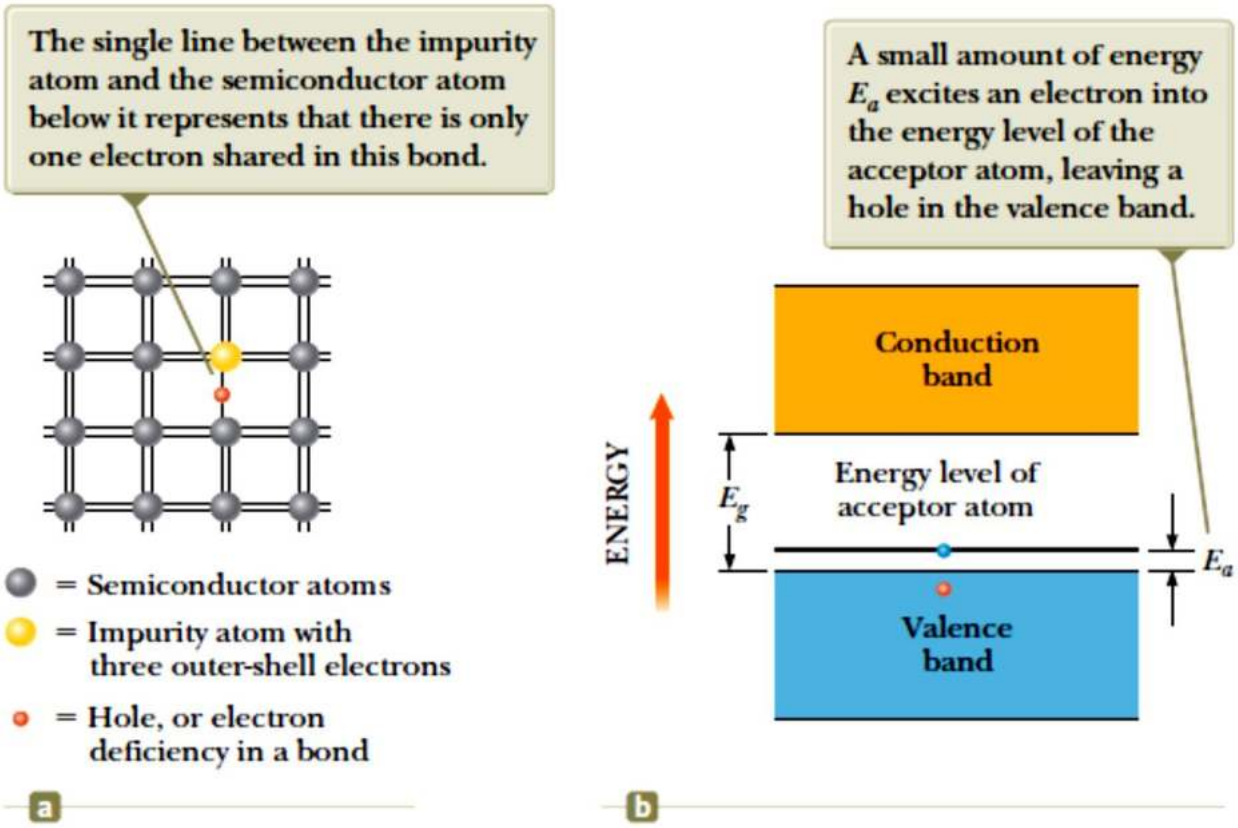
IV semiconductor, four of the electrons form covalent bonds with atoms of the semiconductor and one is left over.



This extra electron is nearly free of its parent atom and can be modeled as having an energy level that lies in the energy gap, immediately below the conduction band. Such a pentavalent atom in effect donates an electron to the structure and hence is referred to as a donor atom. Because the spacing between the energy level of the electron of the donor atom and the bottom of the conduction band is very small (typically, approximately 0.05 eV), only a small amount of thermal excitation is needed to cause this electron to move into the conduction band. (Recall that the average energy of an electron at room temperature is approximately $k_BT \approx 0.025$ eV.) **Semiconductors doped**

with donor atoms are called **n-type semiconductors** because the majority of charge carriers are electrons, which are negatively charged.

If a Group IV semiconductor is doped with atoms containing three outer-shell electrons, such as indium and aluminum, the three electrons form covalent bonds with neighboring semiconductor atoms, leaving an electron deficiency (a hole) where the fourth bond would be if an impurity-atom electron were available to form it.

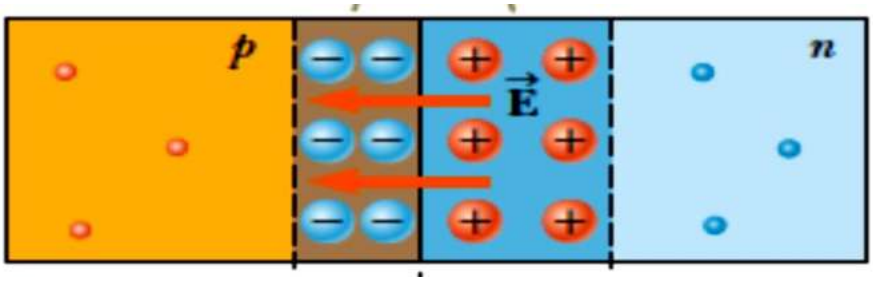


This situation can be modeled by placing an energy level in the energy gap, immediately above the valence band. An electron from the valence band has enough energy at room temperature to fill this impurity level, leaving behind a hole in the valence band. This hole can carry

current in the presence of an electric field. Because a trivalent atom accepts an electron from the valence band, such impurities are referred to as acceptor atoms. **A semiconductor doped with trivalent (acceptor) impurities** is known as **a p-type semiconductor** because the majority of charge carriers are positively charged holes.

The Junction Diode:

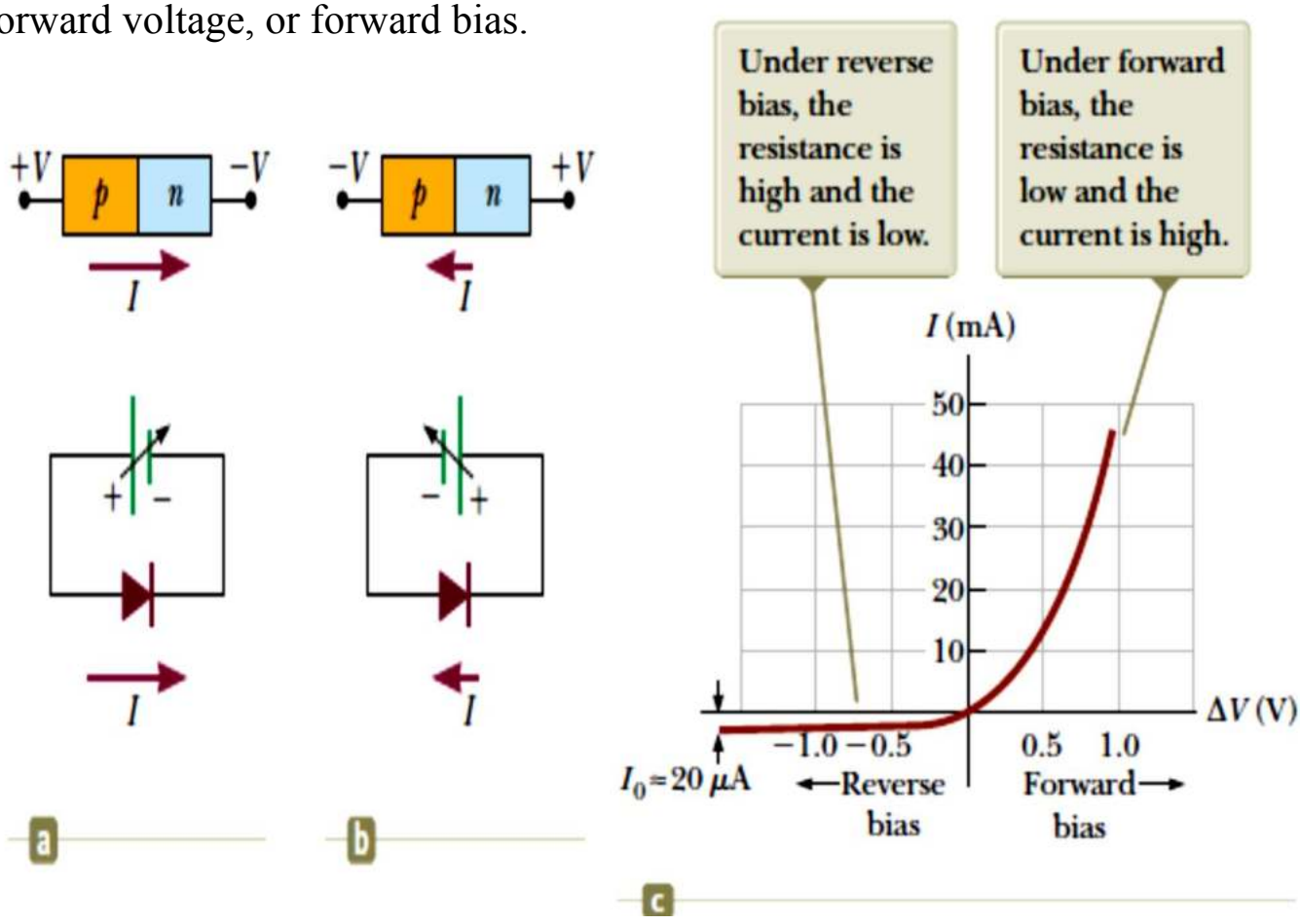
A fundamental unit of a semiconductor device is formed when a p-type semiconductor is joined to an n-type semiconductor to form a p–n junction. **A junction diode is a device that is based on a single p–n junction. The role of a diode of any type** is **to pass current in one direction but not the other.** The p–n junction consists of two distinct regions: a p region, and an n region, a small area that extends several micrometers to either side of the interface, called **a depletion region** which arises when the two halves of the junction are brought together.



The mobile n-side donor electrons nearest the junction diffuse to the p-side and fill holes located there, leaving behind immobile positive ions. While this process occurs, we can model the holes that are being filled as diffusing to the n side, leaving behind a region of fixed negative

ions. This process continues until an internal potential difference ΔV_0 arises in the middle between the two regions (the depletion region) that prevents further diffusion of holes and electrons across the junction and thereby ensures zero current in the junction when no potential difference is applied.

If a voltage ΔV is applied to the junction such that the p-side is connected to the positive terminal of a voltage source as shown in Figure a, the internal potential difference ΔV_0 across the junction decreases; the decrease results in a current that increases exponentially with increasing forward voltage, or forward bias.



For reverse bias (Figure b) (where the n-side of the junction is connected to the positive terminal of a voltage source), the internal potential difference ΔV_0 increases with increasing reverse bias; the increase results in a very small reverse current that quickly reaches a saturation value I_0. The current–voltage relationship for an ideal diode is:

$$I = I_o \left(e^{\frac{e\,\Delta V_o}{k_B\,T}} - 1 \right)$$

where e represents the magnitude of the electron charge, k_B is Boltzmann's constant, and T is the absolute temperature.