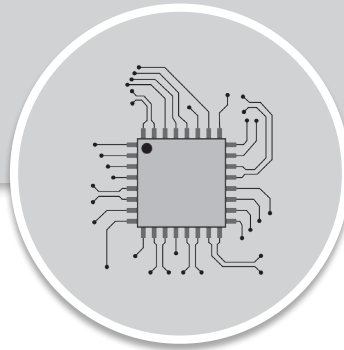


# ELECTRONICS ENGINEERING

## MATERIALS SCIENCE



Comprehensive Theory  
*with Solved Examples and Practice Questions*





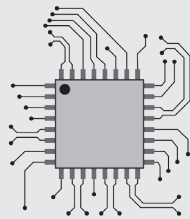
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## **Materials Science**

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# Introduction to Engineering Materials

## 1.1 INTRODUCTION

Material science is a branch of applied science concerned with investigating the relationship existing between the structure of materials and their properties. It is an inter-disciplinary study of materials for entirely practical purposes.

For any kind of product every engineer is vitally concerned with the materials available to him. While making a choice of material for a particular product an engineer must be aware of basic atomic structure of the materials and take into account such properties as strength, electrical conductivity, thermal conductivity, density and others. We shall learn in this set about properties of those materials which have great importance from electrical engineer's point of view.

## 1.2 CLASSIFICATION OF ENGINEERING MATERIALS

From material science point of view materials may be classified under following broad groups:

- (i) Metals and alloys      (ii) Ceramics and glasses      (iii) Organic polymers

- **Metals** are familiar objects with a characteristic appearance; they are capable of changing their shape permanently, and have good thermal and electrical conductivity.
- An **alloy** is a combination of more than one metal.
- **Ceramics and glasses** are non-metallic inorganic substances, which are brittle and have good thermal and electrical insulating properties.
- **Organic polymers** are relatively inert and light, and generally have a high degree of plasticity.

Figure lists typical examples from each of these three groups of materials. In addition, examples of materials which lie between two groups are also shown.

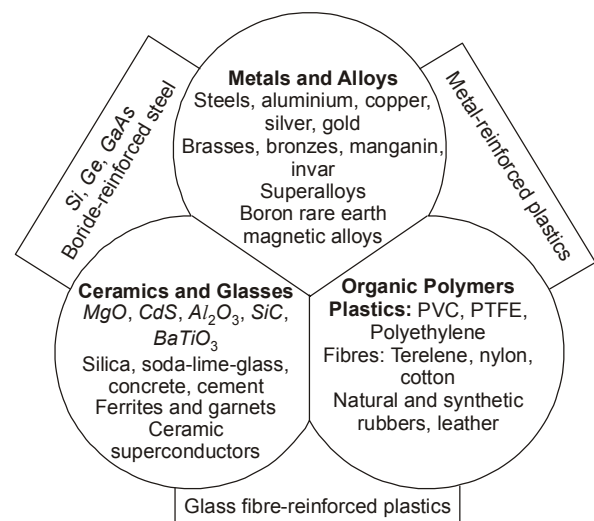


Fig. : Three major groups of engineering materials

## 1.3 CLASSIFICATION OF SOLIDS FROM ELECTRICAL ENGINEERING POINT OF VIEW

From electrical engineering point of view, the materials can be classified as:

(i) conductors    (ii) insulators (dielectrics)    (iii) magnetic materials, and    (iv) semiconductors

### 1.3.1 Conductors

Under a difference of electric potential conductors afford continuous passage of an electric current. Due to flow of current in a conductor some heat is developed which is given by **Joule's Law**. Just like electrical conductivity, the heat conduction in conductors is mostly through free electrons. There exists a relationship between the electrical conductivity and thermal conductivity which is called **Wiedemann Franz Law**.

Some of the good conductors of electricity are silver, copper, aluminium etc.

- Low resistivity metals and alloys are used as conductors and for electrical contacts.
- High resistivity alloys are used for resistors and as heating elements.
- A special class of materials called **superconductors** exhibits almost zero resistivity when they operate below certain temperature – **transition temperature or critical temperature**.

### 1.3.2 Dielectric Materials (Insulating Materials)

These materials provide electrical insulation between two media which are at different potential and also act as stores of electrical charges (in capacitors). When the main function is insulation, the materials are called **insulating materials**, and when charge storage is the main function they are termed as **dielectrics**.

A large number of gaseous, liquid and solid insulating materials are available these days with excellent properties.

### 1.3.3 Magnetic Materials

Magnetic materials are the materials which can become magnets or are attracted towards magnets. Magnetic materials generate electric power, energize electric motors, reproduce sound and visual images and store information in computers, etc.

Of the pure element, only iron, cobalt, nickel and gadolinium are known to be magnetic in the sense at ordinary temperature. The desired properties in magnetic materials can be obtained by a combination of these metals with other elements to form alloys which generally have to be subjected to certain heat treatment to bring about the desired result.

### 1.3.4 Semiconductors

Semiconductors are a class of materials whose electrical conductivity is intermediate between that of a conductor and an insulator. Semiconductors have resistivities that are highly sensitive to temperature and impurity content. Silicon and Germanium are the best known semiconductor materials, have structures which are almost perfect. Some other semiconducting materials are selenium, gray tin, tellurium, etc. Some examples of magnetic semiconductors are NiO, LaMnO<sub>3</sub>, CdCr<sub>2</sub>Se<sub>4</sub>, etc.

## 1.4 THE ATOMIC AND ELECTRONIC STRUCTURE

Recall that every atom consists of a central nucleus surrounded by one or more orbital electrons. Nucleus is composed of protons and neutrons (collectivity known as nucleons). The number of positive charges on the nucleus of an atom always equals the number of orbital electrons, and is called the **atomic number** of the element. **Atomic weight (M)** of the atoms are related to the sum of number of protons and neutrons. But this number physically corresponds to the actual weight of an atom.

## 1.5 QUANTIZED ENERGIES

Recall that a basic law of quantum theory reveals that the energies of particles and waves can assume only certain fixed or quantized values.

For photons, the energy ( $E$ ) is given by,

$$E = h\nu = \frac{hc}{\lambda} \quad \dots(1.1)$$

where,

$h$  = Planck's constant =  $6.62 \times 10^{-34}$  Js

$c$  = Speed of light =  $2.998 \times 10^8$  m/s

$\lambda$  = Wavelength

⇒ Energy levels ( $E_n$ ) are given by the Bohr's theory as,

$$E_n = -\frac{13.6}{n^2} \text{ eV} \quad \dots(1.2)$$

where,

$n$  = states = 1, 2, 3, 4,.....

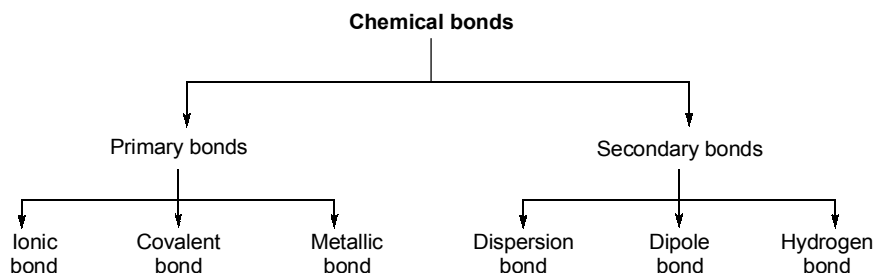
The closer they are to the nucleus, the lower the energies of the electrons.

## 1.6 BONDING IN SOLIDS

### 1.6.1 Chemical Bonding

- The atoms and molecules are held together by strong mutual forces of attraction. These interatomic forces are electrostatic in nature and depend upon the electronic structure of the element.

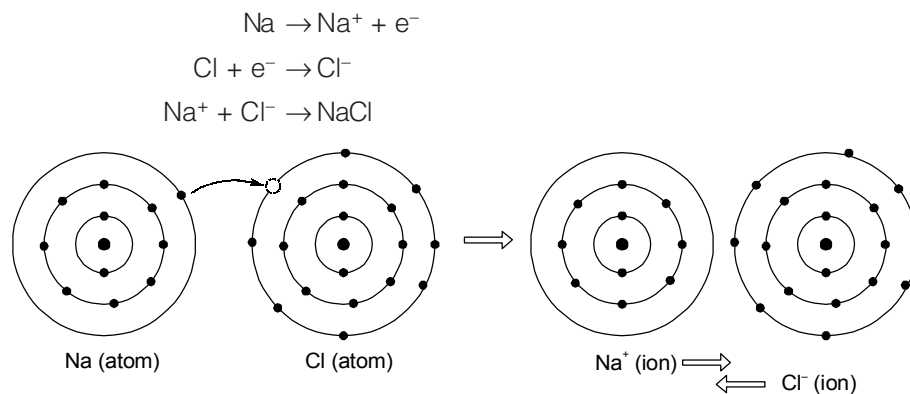
***"Binding forces between atoms and molecules are known as chemical bonds."***



- Primary bonds are interatomic bonds; these bonds are stable and strong.
- Secondary or molecular bonds are formed due to intermolecular attraction forces or vander Waals forces between molecules.
- The atoms or molecules which have their outermost shells completely filled have no tendency to gain, lose or share valence electrons. They have to depend upon Van der Waal's forces of attraction for bonding.
- Van der Waal's forces are due to the electrostatic attraction between nucleus of one atom and the electrons of the other atoms. These bonds are weak and unstable.

### 1.6.2 Ionic Bond

- An ionic bond is formed due to the attractive force between a positive ion and a negative ion when they are brought into close proximity.
- The ions are formed when the atoms involved either lose or gain electrons to stabilize their outer shell electronic configuration by forming ions. Electropositive elements tend to lose electrons while electronegative elements tend to gain electrons.
- The sodium (metal) has a single electron in the outer shell and it tends to lose it, thereby forming a positive ion ( $\text{Na}^+$ ). The chlorine (non-metal) has seven electrons in the outer shell and it tends to gain a single electron for gaining stable configuration, thereby forming a negative ion ( $\text{Cl}^-$ ).
- The positive ions and negative ions attract each other and bonds are formed by the electrostatic binding force as shown below in figure. The chemical reaction can be given as:



**Fig. :** Ionic bond by electrostatic binding force

- Ionic bonds are non-directional and they form compounds which have general characteristics as given below:
  - (i) Crystalline in nature
  - (ii) High strength
  - (iii) High hardness
  - (iv) Having high melting and boiling temperature due to strong electrostatic forces binding atoms.
  - (v) Have brittleness
  - (vi) Non-conducting of electricity

#### Ionic Radius:

- The removal of an electron from an atom results in the formation of a cation while gain of an electron leads to the formation of an anion.
- The ionic radii can be estimated by measuring the distances between cations and anions in ionic crystals.
- The size of an anion will be larger than the parent atom due to the addition of one or more electron will result in increased repulsion among the electrons and a decrease in effective nuclear charge.
- A cation is smaller than its parent atom because it has lesser electrons while its nuclear charge remains the same.

**EXAMPLE : 1.1**

**Explain why cations are smaller and anions are larger in radii than their parent atoms?**

**Solution :**

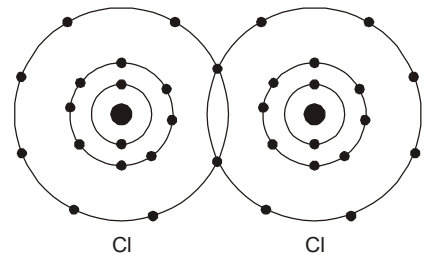
Cations are smaller in size because they are formed by loss of electrons and anions are larger in size because they are formed by the gain of electrons.

**OR**

- Anions are always larger than their parent atoms because the addition of one or more electrons would result in increased repulsion among the electrons and a decrease in the effective nuclear charge. This is opposite in case of cations.
- Cations are always smaller than their parent atoms because they have lesser electrons, whereas their nuclear charge remains the same. The remaining electrons are, therefore held more tightly by the protons in the nucleus and thus their radii are smaller than the parent atoms.

**1.6.3 Covalent Bond**

- A covalent bond is formed by sharing of electrons between the atoms. The covalent bonds are formed between many non-metallic elements as the atoms of these elements, usually have incompletely filled outer electron orbits. Such elements are hydrogen, carbon, chlorine, nitrogen and oxygen.
- The formation of chlorine molecule by covalent bond is shown in figure. The outer shell of chlorine atom has seven electrons. When two chlorine atoms are brought closer, then each chlorine atom tries to gain one electron to form stable electronic configuration. This is achieved by a pair of chlorine atoms by sharing two electrons, thereby producing a stable diatomic molecule.
- Covalent bonds are directional in nature and covalent compound can be solids, liquids and gaseous. The compounds having covalent bond have following general characteristics:
  - (i) Like the ionic bond, the covalent bond tends to produce materials with high strength.
  - (ii) Have high melting and boiling temperature.
  - (iii) Atom movement within the material (deformation) requires the breaking of distinct bonds, thereby making the material characteristically brittle.
  - (iv) Electrical conductivity depends upon the bond strength, ranging from conductive tin (weak covalent bond) through semiconductive silicon and germanium to insulating diamond.
  - (v) Covalent solids do not form closed pack structures as bonding has directional nature.



**Fig. :** Formation of a covalent bond (chlorine molecule)

**Types of Covalent Bond**

**$\sigma$ -(Sigma) bond**

- It follows axial overlapping of orbitals. Bond formed by linear overlapping of half filled atomic orbital is called as sigma bond. A covalent bond results from the formation of a molecular orbital by the end-to-end overlap of atomic orbitals, denoted by the symbol  $\sigma$ , i.e.,  $s$ ,  $p$  along the same axis.

**$\pi$  bond**

- Lateral overlapping of orbitals. It can be formed by overlapping of two adjacent half filled orbitals. When two orbital overlapping form  $\pi$  bond then at the time of overlapping these two orbitals form parallel axis to each other. A covalent bond resulting from the formation of a molecular orbital by side-to-side overlap of atomic orbitals along a plane perpendicular to a line connecting the nuclei of the atoms, denoted by the symbol  $\pi$ , i.e., only  $p$  orbital forms it at the angle called bond angle.
- Hybrid bonds are formed when interaction between  $s$  and  $p$  sub orbitals occur. Double & triple bonds are unsaturated while single bonds are saturated.

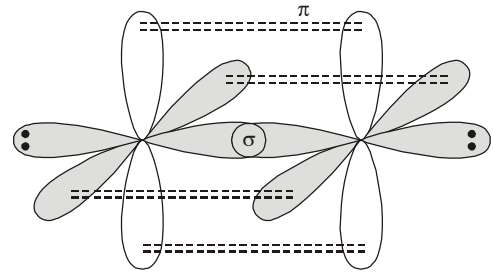


Fig. : Orbital structure of CO

**Covalent Radius**

- Covalent bond radius refers to half of the distance between two singly bonded atoms of the same element or we can define it as half the covalent bond length when the two atoms bonded are homonuclear.  $r_{\text{cov}}$  is typically measured by X-ray diffraction.

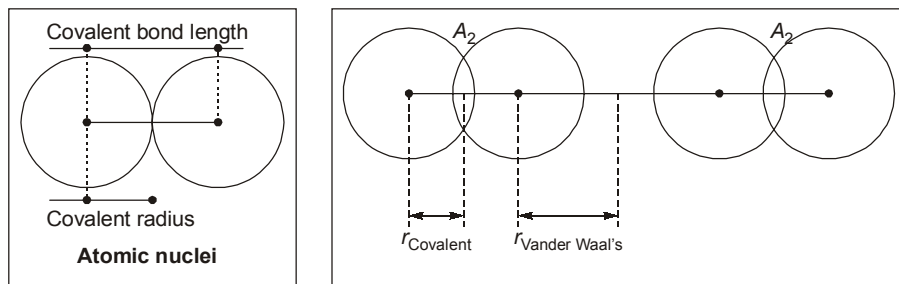


Fig. : Covalent Radius

**1.6.4 Metallic Bond**

- A metallic bond is formed by the partial sharing of valence electrons by the neighbouring atoms. The atoms in metals and alloys are held together by such bonds. The elements having small number of loosely held valence electrons can easily release these electrons to the common pool.
- The bonding takes place when each atom contributes its valence electrons to the formation of an electron cloud and change into positive ions. The valence electrons are no longer bonded directly to any individual atom but they move freely in the sphere of influence of other atoms.
- It means that valence electrons are bonded to different atoms at different times and this binding lasts for a short time.
- Metallic bonding constitutes the electrostatic attraction forces between the delocalized electrons (electron cloud) and the positively charged metal ions.
- Bonding can be understood as the sharing of free electrons among a lattice of positively charged ions (cations). In metallic bonding, electrons are released from atoms, thereby leaving metal cations surrounded by a "sea of delocalized electrons" as shown above in figure.

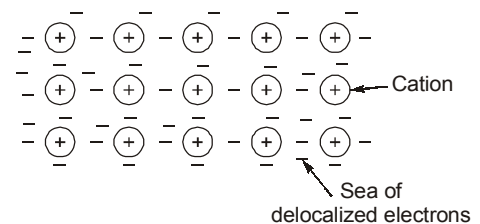


Fig. : Metallic bonding

- The metallic bonding in metals and alloys provides the properties as per table given below.

**Table : Related metal properties due to metallic bonding**

	Property	Explanation
1.	Electrical conductivity	Electrons are free to move through cations lattice, thereby providing electricity carrier.
2.	Lustre	Light is reflected by the sea of delocalized electrons, thereby metal shines, i.e., it has lustre.
3.	Malleability and ductility	Metallic bonding is non-directional. Lattice of cations can be deformed and mobile electrons continue to hold the metal structure together.
4.	High melting and boiling points	Attraction between cation and electron cloud is strong.
5.	High density	Cations are closely packed in a three-dimensional network.

### 1.6.5 Comparison of Primary Bonds

The comparison of primary bonds is as per table given below :

**Table : Comparison of primary bonds**

S.No.	Characteristics	Ionic bond	Covalent bond	Metallic bond
1.	Bond energy	Higher than metallic	Higher than metallic	Generally lower than other primary bonds
2.	Nature of bond	Non-directional	Directional	Non-directional
3.	Examples	NaCl, MgO and CaF <sub>2</sub>	Diamond, silicon germanium etc.	Molecules of Al, Cu, Mg and Ag
4.	Bond formation	Transfer of electrons	Sharing of electrons	Formation of electron cloud and cations
5.	Bonding force	Electrostatic force between anions and cations	Electrostatic force of attraction between two atoms	Electrostatic force between electron cloud and cations
6.	Conductivity	Low	Moderate	High
7.	Melting and boiling temperature	High	High	High
8.	Mechanical properties	High hardness	Hard	Good strength and ductility

### 1.6.6 Van der Waal Bond

- Van der Waals bond exists between two closed configuration atoms or between molecules and it is relatively a weak bond. The bond is due to dipole-dipole interaction.
- Van der Waals forces are a result of electrostatic attraction between temporary dipoles and induced dipoles caused by motion of electrons in atoms and molecules.
- Van der Waals forces are forces that occur between molecules of the similar substance. They are quite different from the forces that make up the molecule.
- The strength of Van der Waals forces is related to the size of atoms and molecules. Bigger the atom or molecule responds to the bigger Van der waals force.

#### Atomic Radius:

- It is generally stated as the total distance from an atom's nucleus to the outermost orbital of electron.
- In simpler terms, it can be defined as something similar to the radius of a circle, where the centre of the circle is the nucleus and the outer edge of the circle is the outermost orbital of electron.
- Atomic radius is measured in picometers (pm) or angstroms (Å).

- An atom gets larger or the radius of atoms increases as the number of electronic shells increase; therefore the radius of atoms increases as you go down in a certain group in the periodic table of elements.
- In general, the size of an atom will decrease as you move from left to the right of a certain period.

### Van der Waal Radius:

It is defined as half of the inter nuclear separation of two non-bonded atoms of the same element on their closest possible approach and is denoted by  $r_v$ .

### 1.6.7 Dispersion Bonds

- In a symmetrical molecule, the electrons are distributed uniformly around the nucleus and the electrons are constantly rotating about nucleus. In a symmetrical molecule, the centres of positive charges and negative charges coincide with each other.
- However, in molecules where the distribution of electrons is not symmetrical about their nuclei. This causes the displacement between the centres of positive and negative charges as shown below in figure.
- It creates electronic imbalance of the charge and this is called polarization. This polarization fluctuates with motion of electrons and is known as dispersion effect.
- Dispersion effect produces a weak force of attraction between two molecules of the same element and this bonding is called dispersion bond. Such bond is found in noble gases like argon, helium and neon etc.

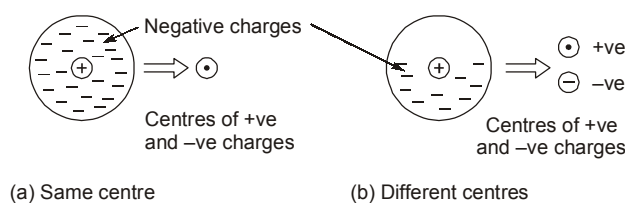


Fig. : Dispersion effects

### 1.6.8 Dipole Bonds

- In covalent bonding, there may be unequal sharing of electrons between two atoms forming molecules. This happens if one of the atoms has high affinity to attract electrons than the other atoms.
- The unequal sharing of electrons creates opposite charges on the molecules. As a result, permanent dipoles are produced. These dipoles attract each other, thereby forming dipole bonds.
- Dipole bonds are weaker than primary bonds but they are stronger than dispersion bonds.
- Hydrogen fluoride molecule has dipole bond as shown below in figure.
- Fluorine atom has higher affinity than the hydrogen atom. Due to this, the shared electron pair shifts towards the fluorine atom in the covalent bonding. The shifting of electron pair produces a dipole with positive charge towards hydrogen atom and negative charge towards fluorine atom. The resulting dipoles produce necessary attraction to produce dipole bonding of molecules.

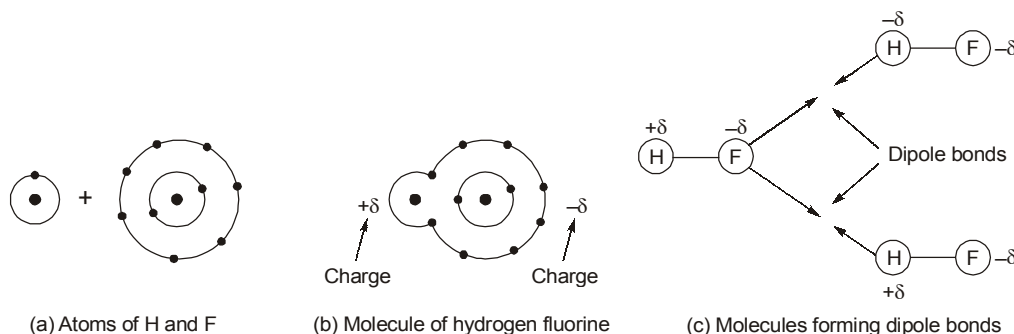


Fig. : Formation of dipole bonds



**OBJECTIVE  
BRAIN TEASERS**

- Q.1** The Miller indices are same for  
 (a) perpendicular planes  
 (b) crystal planes  
 (c) parallel planes  
 (d) three crystallographic axes
- Q.2** When *BCC* iron is heated, it changes to *FCC* iron resulting in  
 (a) increase in volume of unit cell  
 (b) contraction in volume of unit cell  
 (c) no change in volume of unit cell  
 (d) cracks in the material
- Q.3** A crystal lattice, the vacancies created by the absence of certain atoms are known as  
 (a) Hertz defect (b) Pauli's defect  
 (c) Frankel defect (d) Schottky defect
- Q.4** Consider the following statements with regard to *FCC* structure:  
 1. Number of nearest neighbour atoms is twelve.  
 2. Packing efficiency is 0.74.  
 3. There is an atom at the body centre of the unit cell.
- Which of the statements given above is/are correct?  
 (a) 1, 2 and 3 (b) 1 and 2  
 (c) 2 and 3 (d) 1 and 3
- Q.5** The atomic packing factor for body centric cubic is  
 (a) 0.52 (b) 0.62  
 (c) 0.68 (d) 0.74
- Q.6** Match **List-I** (Atoms) with **List-II** (Corresponding Cubic Crystal Structure) and select the correct answer using the codes given below the lists:

**List-I :**

- A.** Silicon  
**B.** Gold  
**C.** Magnesium  
**D.** Maganese

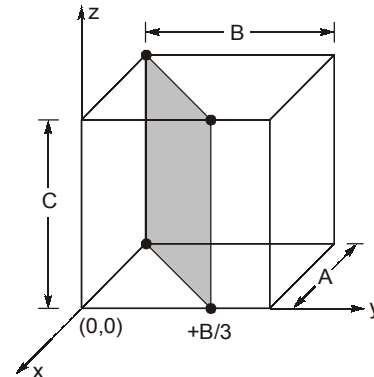
**List-II :**

1. Simple cubic structure
2. Body centered cubic structure
3. Face centered cubic structure
4. Diamond cubic structure
5. Hexagonal closed packing

**Codes:**

	A	B	C	D
(a)	4	3	5	1
(b)	3	4	2	5
(c)	1	2	3	4
(d)	5	3	4	2

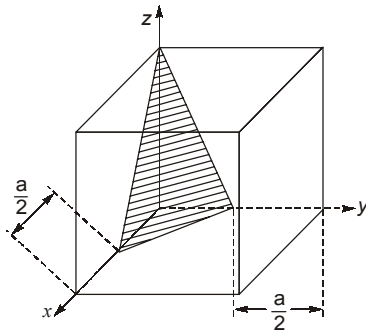
- Q.7** Miller indices of the shaded figure in structure given below is



- (a)  $+A, \frac{B}{3}, C$  (b)  $-1, \frac{1}{3}, \infty$   
 (c)  $-A, \frac{B}{3}, \infty$  (d)  $-1, 3, 0$

- Q.8** The unit cell of a certain type of crystal is defined by 3 vectors  $\vec{a}, \vec{b}$  and  $\vec{c}$ . The vectors are mutually perpendicular but  $a = b \neq c$ . The crystalline structure is  
 (a) Triclinic (b) Tetragonal  
 (c) Monoclinic (d) Orthorhombic
- Q.9** In a silicon crystal, the arrangement of atoms repeats periodically. This type of material is classified as  
 (a) Amorphous and non-crystalline  
 (b) Non-crystalline and epitaxial  
 (c) Epitaxial and single crystal  
 (d) Amorphous and single crystal

- Q.10** Each side of the cube shown below is of length  $a$ . What are the Miller indices of the shaded surface?



- (a) (100)                      (b) (123)  
(c) (221)                      (d)  $\left(\frac{1}{2} \frac{1}{2} 1\right)$

- Q.11** Consider the following statements regarding forms of carbon:

1. Graphite has three coplanar covalent bonds in its structure.
2. Packing of atoms in diamond is such that has a very low packing efficiency.
3. There exists a Vander Waal's interaction between two layers of graphite.

Which of the above given statements are correct?

- (a) 1 and 2 only              (b) 1 and 3 only  
(c) 2 and 3 only              (d) 1, 2 and 3

- Q.12** Unit cell edge length (a) for BCC unit cell is (radius of each atom is  $R$ )

- (a)  $\frac{4R}{\sqrt{3}}$                       (b)  $2\sqrt{2}R$   
(c)  $\frac{\sqrt{3}}{4}R$                       (d)  $3\sqrt{2}R$

- Q.13** Lattice constants and angles of Triclinic crystal are

- (a)  $a = b = c, \alpha = \beta = \gamma \neq 90^\circ$ .  
(b)  $a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$ .  
(c)  $a \neq b \neq c, \alpha = \gamma = 90^\circ \neq \beta$ .  
(d)  $a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^\circ$ .

- Q.14** Atomic packing factor for body centered cubic and diamond cubic crystal structure are respectively

- (a) 0.52 and 0.68              (b) 0.68 and 0.74  
(c) 0.52 and 0.74              (d) 0.68 and 0.34

- Q.15** Consider the following statements regarding electronic polarization:

1. This polarization occurs in materials containing non-polar molecules and monatomic gas.
2. This polarization causes displacement in negatively charged electron cloud.
3. The electronic polarization is dependent on temperature.

Which of the above given statements are correct?

- (a) 1 and 2 only              (b) 2 and 3 only  
(c) 1 and 3 only              (d) 1, 2 and 3

- Q.16** The distance between the two atoms of basis of a diamond structure if the value of lattice constant of the structure is  $8\text{\AA}$  will be

- (a)  $1.73\text{\AA}$                       (b)  $2.42\text{\AA}$   
(c)  $1.21\text{\AA}$                       (d)  $3.46\text{\AA}$

- Q.17** Consider the following statements:

1. The smallest group of atoms which when repeated regularly form crystal is called space lattice.
2. A closed packed hexagonal space lattice is found in chromium and molybdenum.
3. The atomic packing fraction of BCC structure is near by 0.68.

Which of the above given statement(s) is/are **not** correct?

- (a) 1 and 3 only              (b) 1 only  
(c) 1 and 2 only              (d) 2 only

- Q.18** Consider the following statements:

1. An increase in BCC iron volume is observed when heated due to change of BCC iron to FCC iron.
2. If the dislocation density in the crystal is high, it results in high mechanical strength of crystal.
3. Ionic crystals are hard and corrosive both in nature.

Which of the above given statements are correct?

- (a) 1 and 2 only              (b) 1 and 3 only  
(c) 2 and 3 only              (d) 1, 2 and 3

**ANSWERS KEY**

1. (c)    2. (b)    3. (d)    4. (b)    5. (c)  
6. (a)    7. (d)    8. (b)    9. (c)    10. (c)  
11. (d)    12. (a)    13. (d)    14. (d)    15. (a)  
16. (d)    17. (c)    18. (b)

**HINTS & EXPLANATIONS**

**1. (c)**

The number of open-loop poles in RHS are  $P=0$ .

**2. (b)**

APF of BCC = 0.68

APF of FCC = 0.74

and  $APF \propto \frac{1}{\text{Volume of unit cell}}$

**4. (b)**

In FCC structure, there are atoms at the centre of each face and at every corner.

**7. (d)**

Intercepts made by plane on 3 axis

$$\Rightarrow -A, \frac{B}{3}, \infty$$

$\therefore$  Miller indices

$$\Rightarrow -1, 3, 0$$

**9. (c)**

A crystal has periodicity of atoms.

**11. (d)**

All of the above statements are correct.

**15. (a)**

Electronic polarization is independent of temperature.

**16. (d)**

Given lattice constant  $a : 8 \text{ \AA}$

Distance between the two atoms is equivalent to nearest neighbour distance

For diamond structure

$$\text{Nearest neighbour distance} = \frac{\sqrt{3}}{4}a$$

Distance between two atoms

$$= \frac{\sqrt{3}}{4} \times 8 = 2\sqrt{3} \text{ \AA} = 3.46 \text{ \AA}$$

**17. (c)**

- The smallest group of atoms which when repeated regular to form crystal is unit cell.
- Closed hexagonal space lattice is found in Cobalt, antimony and bismuth.

**18. (b)**

If dislocation density is high, mechanical strength of material decreases.



**CONVENTIONAL BRAIN TEASERS**

**Q1** Molybdenum has the BCC crystal structure, a density of  $10.22 \text{ g cm}^{-3}$  and an atomic mass of  $95.94 \text{ g mol}^{-1}$ . Find the atomic concentration, lattice parameter  $a$ , and atomic radius of molybdenum?

**1. (Sol.)**

- Since molybdenum has BCC crystal structure, there are 2 atoms in the unit cell.

- The density can be given by,

$$\rho = \frac{\text{Mass of atoms in unit cell}}{\text{Volume of unit cell}} = \frac{(\text{Number of atoms in unit cell}) \times (\text{Mass of one atom})}{\text{Volume of unit cell}} = \frac{2 \left( \frac{M_{at}}{N_A} \right)}{a^3}$$

$$\text{So, } a = \left( \frac{2M_{at}}{\rho N_A} \right)^{1/3} = \left( \frac{2 \times 95.94}{10.22 \times 6.022 \times 10^{23}} \right)^{1/3} \text{ cm} = 3.147 \times 10^{-10} \text{ m}$$

- Since, there are 2 atoms in a cube of volume  $a^3$ . Hence, the atomic concentration ( $n_{at}$ ) is

$$n_{at} = \frac{2}{a^3} = \frac{2}{(3.147 \times 10^{-10})^3} \text{ m}^{-3} = 6.415 \times 10^{28} \text{ m}^{-3}$$

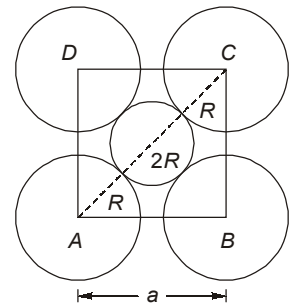
- For a BCC cell, the lattice parameter  $a$  and the radius of the atom  $R$  are related by,

$$R = \frac{a\sqrt{3}}{4} = \frac{(3.147 \times 10^{-10})\sqrt{3}}{4} \text{ m} = 1.363 \times 10^{-10} \text{ m}$$

**Q2** Consider the FCC unit cell of the copper crystal shown in figure below:

- How many atoms are there per unit cell?
- Calculate the lattice parameter ' $a$ ' if  $R$  is the radius of Cu atom.
- Calculate the atom packing fraction.
- Calculate the atomic concentration in Cu crystal and the density of the crystal given that the atomic mass of Cu is  $63.55 \text{ g mol}^{-1}$  and the radius of the Cu atom is  $0.125 \text{ nm}$ .

(Assume lattice parameter,  $a = 0.362 \text{ nm}$ )



**2. (Sol.)**

- The Cu atom at each corner is shared with eight other adjoining unit cells. Each Cu atom at the face center is shared with the neighbouring unit cell. Thus, the number of atoms per unit cell

$$= 8 \text{ corner} \left( \frac{1}{8} \text{ atom} \right) + 6 \text{ faces} \left( \frac{1}{2} \text{ atom} \right) = 4 \text{ atoms}$$

- Consider the unit cell given and one of the cubic faces. The face is a square of side  $a$  and the diagonal is  $\sqrt{a^2 + a^2} = a\sqrt{2}$ .

The diagonal has one atom at the center of diameter  $2R$ , which touches two atoms centered at the corners.

The diagonal, going from corner to corner is therefore  $R + 2R + R$ . Thus  $4R = a\sqrt{2}$ .

$$\therefore a = \frac{4R}{\sqrt{2}} = 2\sqrt{2}R$$

- Atomic packing fraction (APF)

$$= \frac{(\text{Number of atoms in unit cell}) \times (\text{Volume of atom})}{\text{Volume of unit cell}} = \frac{4 \times \frac{4}{3} \pi R^3}{a^3} = \frac{\frac{16}{3} \pi R^3}{(R2\sqrt{2})^3} = \frac{16\pi}{3(2\sqrt{2})^3}$$

$$\therefore \text{APF} = 0.74$$