

# Electronics Engineering

# Materials Science

Comprehensive Theory

*with* Solved Examples and Practice Questions



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**Materials Science**

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First Edition : 2015

Second Edition : 2016

Third Edition : 2017

Fourth Edition : 2018

Fifth Edition : 2019

Sixth Edition : 2020

Seventh Edition : 2021

Eighth Edition : 2022

**Ninth Edition : 2023**

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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.

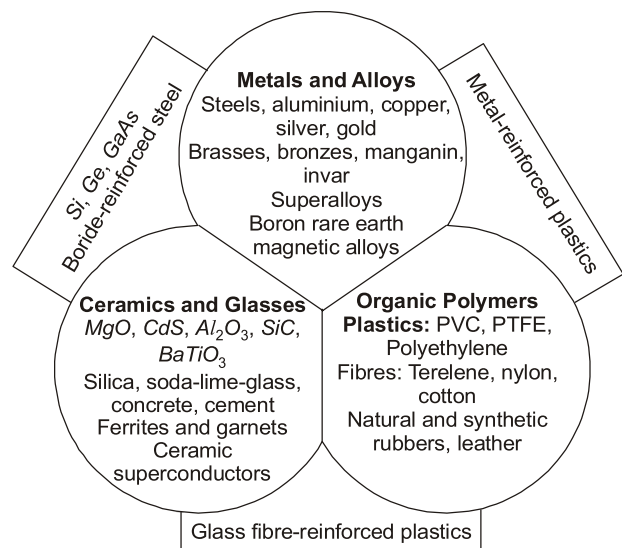
For any kind of product every engineer is vitally concerned with the materials available to him. While making a choice of material for a particular product an engineer must be aware of basic atomic structure of the materials and take into account such properties as strength, electrical conductivity, 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. 1.1 : 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  $\text{NiO}$ ,  $\text{LaMnO}_3$ ,  $\text{CdCr}_2\text{Se}_4$ , 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.

Here in this set writer assumes that readers are well known with the atomic and electronic structure, so much importance is not given to the concerned topic.

## 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

$\Rightarrow$  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

Atoms are rarely found as free and independent units, but usually are linked or bonded to other atoms in some manner as a result of interatomic forces. These binding forces between the atoms are called chemical bonds. According to the strength, chemical bonds are grouped into **Primary** and **Secondary bonds**. The primary bonds are interatomic bonds, where as the secondary bonds are inter molecular bonds. The primary bonds are stronger than the secondary bonds.

There are basically four classes into which the bonds can conveniently be divided, although the boundaries between them are not always distinct:

- (i) ionic bonding
- (ii) covalent bonding
- (iii) metallic or unsaturated covalent bonding, and
- (iv) Vander Waal's bonding.

The first three are primary bonds, whereas the fourth one is a secondary bond.

## 1.7 Atom Arrangement in Materials

Properties of materials are highly influenced by arrangement of atoms. Depending upon the manner of atomic grouping, materials are classified as having **molecular structures**, **crystal structures** and **amorphous structures**. Typical examples of molecules include  $O_2$ ,  $H_2O$  and  $C_2H_4$ . Glass is an example of amorphous structure.

### 1.7.1 Crystalline Structure of Metals

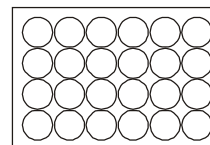
Generally, metals are crystalline and non-metals (Plastic, Ceramics, Rubber etc.) are non-crystalline. But this is not a rule. In crystalline solids the atoms are arranged in a regular geometrical array known as **space lattice**. These lattices are described by a unit building block which is essentially repeated throughout space in a periodic manner. Such blocks are known as unit cells. A crystalline solid can be either a single crystal, where the entire solid consists of only one crystal, or an aggregate of many crystals separated by well-defined boundaries. In the latter form, the solid is said to be **polycrystalline**.

### 1.7.2 Crystallinity

Crystallinity is the property of a solid in which atoms or molecules are arranged in orderly or periodic manner.

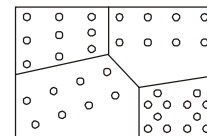
### 1.7.3 Single Crystal

A single crystal material atoms or molecules are arranged in regular or periodic manner. These materials are anisotropic for e.g. Quartz.



### 1.7.4 Polycrystalline

These materials consist of grain within which atomic arrangement is regular but it shows irregularities from one grain to another, because of random distribution of grain these materials are isotropic. e.g. Polycrystalline silicon.



### 1.7.5 Anisotropic and Isotropic Material

- (a) **Anisotropic Material:** If the properties of material depends on the direction in which they are measured then materials are called anisotropic, e.g. Quartz.
- (b) **Isotropic Material:** If the properties of material does not depend on the direction in which they are measured then materials are called isotropic material, e.g. Polycrystalline silicon.

## 1.8 Amorphous

In amorphous structure atoms up to first nearest neighbours are arranged periodically but the atom which are away from nearest atom are found to be arranged randomly.

When the atom are not arranged in a regular manner an amorphous material may be formed. e.g. Supercooled state of  $\text{SiO}_2$  corresponds to glass.

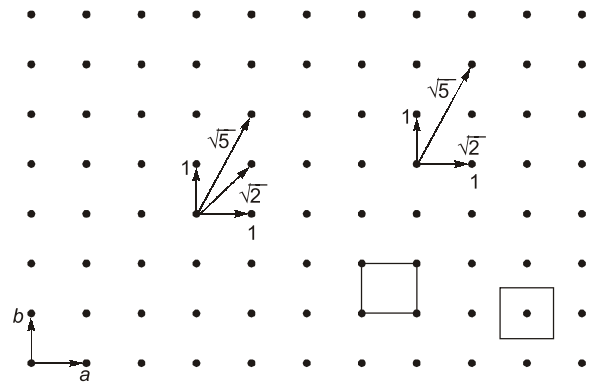
In other cases, the molecule may be extremely long and irregular in shape so that orderly arrangement may not be obtained, e.g. Polymer.

## 1.9 Space Lattice

A space lattice is defined as an infinite array of points in three-dimensional space in which each point is identically located with respect to the other. Concept of space lattice is helpful in understanding the crystal structure of existing materials, and also those materials which are likely to be developed in future. As an example, for ease of representation on paper, consider a two dimensional square array of points shown in figure. By repeated translation of the two vectors  $\vec{a}$  and  $\vec{b}$  on the plane of the paper, we can generate the square array. The magnitudes of  $\vec{a}$  and  $\vec{b}$  are equal and can be taken to be unity. The angle between them is  $90^\circ$ ;  $\vec{a}$  and  $\vec{b}$  are called the **fundamental translation vectors** that generate the square array.



If we locate ourselves at any point in the array and look out in a particular direction that lies on the plane of the paper, the scenery is the same, irrespective of where we are. Consider the immediate surroundings of a point in the array. If we look due north or due east from this point, we see another point at a distance of  $\sqrt{2}$  units and along north-northeast, the nearest point is at a distance of  $\sqrt{5}$  units. As this is true of every point in the array, the array satisfies the definition given above and can be called a two-dimensional square lattice.



A two dimensional square array of points gives a square lattice. Two ways of choosing a unit cell are illustrated

**Fig. 1.2**

## 1.10 Basis

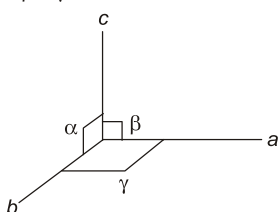
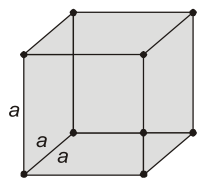
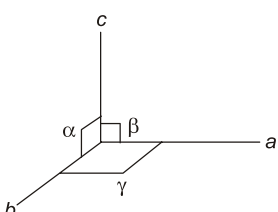
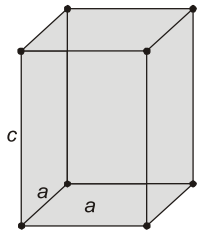
The way of filling-up of points in a space lattice by the atoms is known as **Basis**. Each point may be occupied by one, two or many atoms in different solids. The space lattice when combines with the basis generates a unit cell. Thus,

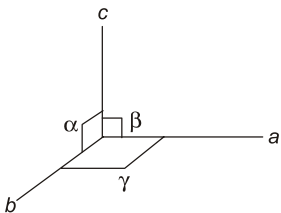
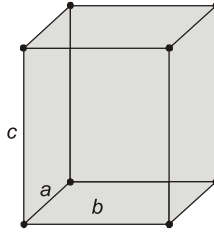
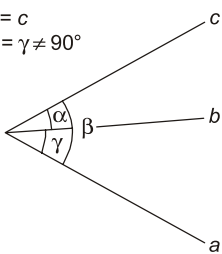
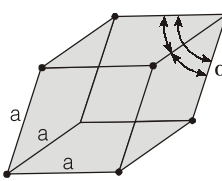
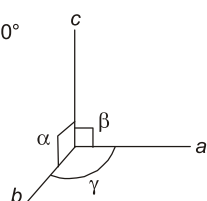
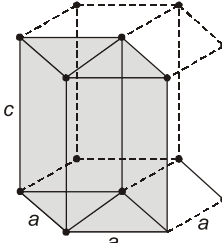
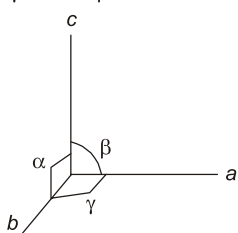
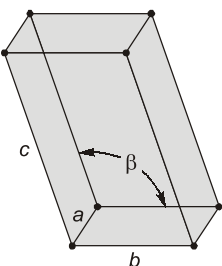
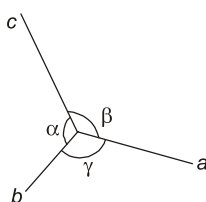
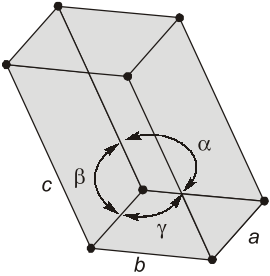
$$\text{Space lattice} + \text{Basis} = \text{Unit cell}$$

## 1.11 Bravais Lattices

A three-dimensional space lattice is generated by repeated translation of three non-coplanar vectors,  $\vec{a}$ ,  $\vec{b}$  and  $\vec{c}$ .

**Table-1.1**

Crystal System	Space Lattice	Unit cell
<b>1. Cubic</b> $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$ 	1. Simple (Lattice points at the eight corners of the unit cell). 2. Body centred (Points at the eight corners and at the body centre). 3. Face centred (Points at the eight corners and at the six face centres).	
<b>2. Tetragonal</b> $a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$ 	4. Simple (Points at the eight corners of the unit cell). 5. Body centred (Points at the eight corners and at the body centre).	

<p><b>3. Orthorhombic</b>  <math>a \neq b \neq c</math>  <math>\alpha = \beta = \gamma = 90^\circ</math></p> 	<p>6. Simple (Points at the eight corners of the unit cell).</p> <p>7. End centred (Also called side centred or base centred) (Points at the eight corners and at two face centre opposite to each other)</p> <p>8. Body centred (Points at the eight corners and at the body centre).</p> <p>9. Face centred (Points at the eight corners and at the six face centres).</p>	
<p><b>4. Rhombohedral or Trigonal</b>  <math>a = b = c</math>  <math>\alpha = \beta = \gamma \neq 90^\circ</math></p> 	<p>10. Simple (Points at the eight corners of the unit cell).</p>	
<p><b>5. Hexagonal</b>  <math>a = b \neq c</math>  <math>\alpha = \beta = 90^\circ</math>  <math>\gamma = 120^\circ</math></p> 	<p>11. Simple          [(i) Points at the eight corners of the unit cell outlined by thick lines or          (ii) Points at the twelve corners of the hexagonal prism and at the centres of the two hexagonal faces].</p>	
<p><b>6. Monoclinic</b>  <math>a \neq b \neq c</math>  <math>\alpha = \gamma = 90^\circ \neq \beta</math></p> 	<p>12. Simple (Points at the eight corners of the unit cell).</p> <p>13. End centred (Points at the eight corners and at two face centres opposite to each other)</p>	
<p><b>7. Triclinic</b>  <math>a \neq b \neq c</math>  <math>\alpha \neq \beta \neq \gamma \neq 90^\circ</math></p> 	<p>14. Simple (Points at the eight corners of the unit cell).</p>	

It so turns out that there are only 14 distinguishable ways of arranging points in three-dimensional space such that each arrangement confirms to the definition of a space lattice. These 14 space lattices are known as **Bravais lattices**, named after their originator. They belong to **seven crystal systems** and are listed in Table (1.1) according to the crystal system.

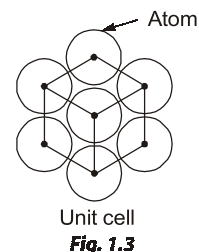
## 1.12 Unit Cell

A unit cell is defined as the basic structure part in the composition of materials.

It is analogous to a brick used in the building construction.

The unit cell will be called monatomic if only one atom occupies a lattice point. When two atoms occupy a lattice point, it will make a dia-atomic unit cell. Similarly the unit cell will be known as multi-atomic when too many atoms occupy a lattice point.

⇒ In 3-Dimensional point of view there are four types of possible unit cells.



### 1.12.1 Primitive (p-type) or Simple Cubic

It has lattice point only at corners and each corner is common in eight cells. So each cell represents a single lattice point as shown in figure (a)

$$\therefore 8 \times \frac{1}{8} = 1 \text{ lattice point/unit cell.}$$

### 1.12.2 Body centered cell (I-type or Incentre type)

It has lattice points at corners as well as at centre of each cell. So each cell has two lattice points per unit cell as shown in figure (b)

$$\text{i.e. } 8 \times \frac{1}{8} + 1 = 2 \text{ lattice points/unit cell, as shown in figure (b).}$$

### 1.12.3 Face centred cell (F-type)

It has lattice points at corners as well as at centre of each face of the cell, as shown in figure (c).

$$\text{i.e. } 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 1 + 3 = 4 \text{ lattice points/unit cell.}$$

### 1.12.4 Base centred (C-type)

It has lattice points at corners as well as at centre of top and bottom face of cell.

It has two lattice points per unit cell as shown in figure (d).

$$\text{i.e. } 8 \times \frac{1}{8} + 2 \times \frac{1}{2} = 1 + 1 = 2 \text{ lattice points/unit cell.}$$

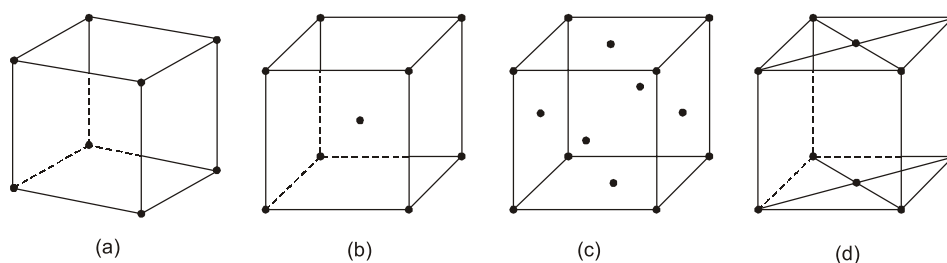
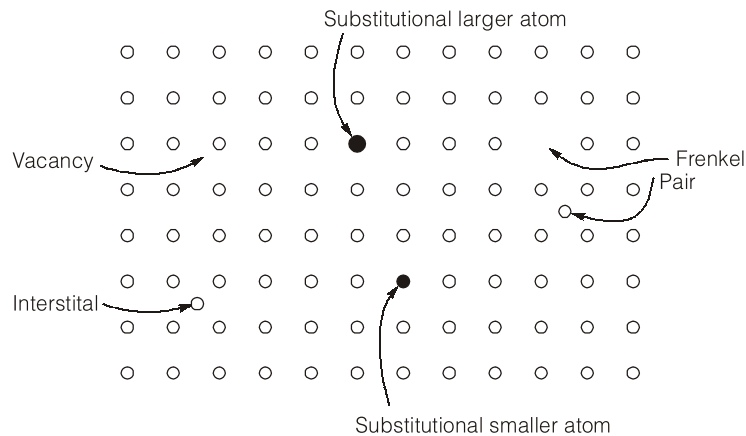


Fig. 1.4



**Fig. 1.14**

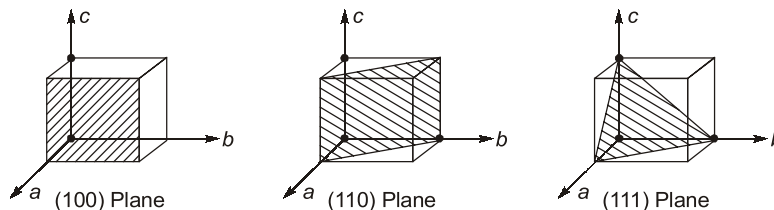
### 1.18.2 Line Defect

Dislocations are linear defects when some of the atoms of the crystal lattice are misaligned. There are two basic types of dislocations, the edge dislocation and the screw dislocation.

**Example - 1.1** Draw sketches illustrating a (100) plane, a (110) plane, and a (111) plane in a cubic unit cell. How many equivalent (100) planes are there in a cubic crystal? A material has a face-centred cubic structure with an ionic radius of 1.06 Å. Calculate the inter planar separation for (111) planes.

[IES : 2004]

**Solution:**



There are six equivalent (100) planes in a cubic crystal.

⇒ In a face-centred cubic structure

$$a\sqrt{2} = 4r$$

where,  $a$  = side of cube  
 $r$  = ionic radius

Given,

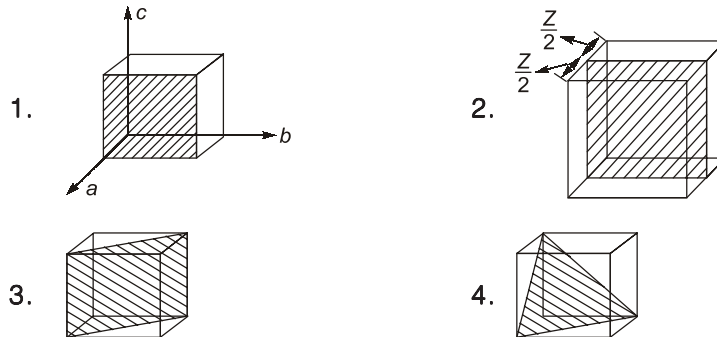
$$r = 1.06 \text{ Å}$$

$$a = \frac{4r}{\sqrt{2}} = \frac{4 \times 1.06}{\sqrt{2}} = 2.998 \text{ Å}$$

Inter planar separation for (111) planes is

$$d = \frac{a}{\sqrt{3}} = \frac{2.998}{\sqrt{3}} = 1.731 \text{ Å}$$

**Example - 1.2** Consider the following crystallographic planes (shaded) using a cube of size  $z$  as shown in the diagram:



Which one of the following gives Miller indices of the above planes, in order?

- (a) (100), (200), (100), (111)      (b) (100), (200), (110), (111)  
(c) (111), (110), (200), (100)      (d) (200), (111), (110), (100)

[ESE : 2004]

Ans. (b)

**Example - 1.3** Which of the following statements is/are true for the diamond structure?

1. Coordination number is four.
  2. Packing fraction is 0.34.
  3. Copper crystallizes into diamond structure.
  4. Lattice is FCC.
- (a) 1 only      (b) 1, 2 and 4  
(c) 2 and 3 only      (d) 2, 3 and 4

[ESE : 2009]

**Solution: (b)**

- (i) The crystal structure of diamond is equivalent to a face-centred cubic (FCC) lattice.
- (ii) In diamond each carbon atom is at the centre of a tetrahedron formed by four other carbon atoms, so the co-ordination number is four.
- (iii) In diamond, each atom can be thought of as a sphere with a radius of  $1/8$  of the cubic body diagonal. Therefore,

$$\text{Packing fraction} = \frac{8 \times \frac{4}{3} \pi r^3}{a^3}$$

where,  $a$  = side of cube  
 $r$  = radius of carbon atom

Here,  $r = \frac{a\sqrt{3}}{8}$

Putting values,  $\text{Packing fraction} = \frac{8 \times \frac{4}{3} \pi \left( \frac{a\sqrt{3}}{8} \right)^3}{a^3} \approx 0.34$



- An electron weighs only  $9.108 \times 10^{-31}$  kg whereas protons and neutrons weigh about **1840 times heavier**.
- When **cooling is fast** we get non-crystalline material and when **cooling is slow** we get, crystalline material.
- When an electron moves towards the nucleus then **energy radiated** and moved away from nucleus, energy will **absorbed** by the electrons.
- In solids the electrons number  $10^{28}/m^3$  and all interact with one another.
- The crystal structure is real whereas lattice is imaginary.
- $(APF)_{DC} < (APF)_{SCC} < (APF)_{BCC} < (APF)_{FCC}$ .
- Epitaxial III - V group semiconductor compounds have **zinc blends** crystal structure.
- Epitaxial II - VI group semiconductor compounds have **Wurwitz** crystal structure.
- **Co-ordination number of diamond crystal is 4.**



### Student's Assignments

- Q.1** The Miller indices are same for
- perpendicular planes
  - crystal planes
  - parallel planes
  - three crystallographic axes
- Q.2** When *BCC* iron is heated, it changes to *FCC* iron resulting in
- increase in volume of unit cell
  - contraction in volume of unit cell
  - no change in volume of unit cell
  - cracks in the material
- Q.3** A crystal lattice, the vacancies created by the absence of certain atoms are known as
- Hurtz defect
  - Pauli's defect
  - Frankel defect
  - Schottky defect
- Q.4** Consider the following statements with regard to FCC structure:
- Number of nearest neighbour atoms is twelve.
  - Packing efficiency is 0.74.
  - There is an atom at the body centre of the unit cell.

Which of the statements given above is/are correct?

- 1, 2 and 3
- 1 and 2
- 2 and 3
- 1 and 3

- Q.5** The atomic packing factor for body centric cubic is

- 0.52
- 0.62
- 0.68
- 0.74

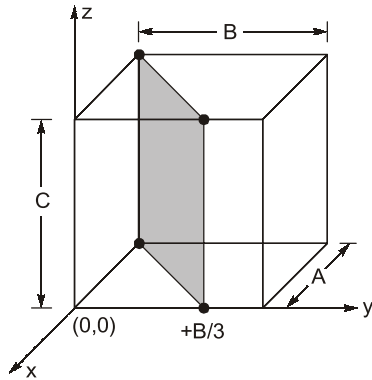
- Q.6** Match **List-I** (Atoms) with **List-II** (Corresponding Cubic Crystal Structure) and select the correct answer using the codes given below the lists:

List-I	List-II
A. Silicon	1. Simple cubic structure
B. Gold	2. Body centred cubic structure
C. Magnesium	3. Face centred cubic structure
D. Manganese	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)  $-1, 3, 0$

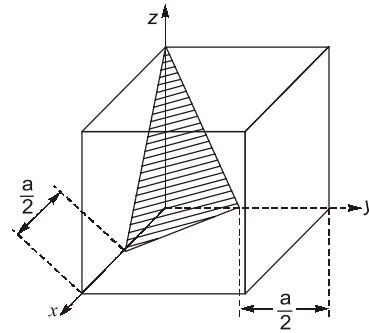
Q.8 The unit cell of a certain type of crystal is defined by 3 vectors  $\vec{a}$ ,  $\vec{b}$  and  $\vec{c}$ . The vectors are mutually perpendicular but  $a = b \neq c$ . The crystalline structure is

- (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)  $\left(\frac{1}{2}, \frac{1}{2}, 1\right)$

#### ANSWERS

1. (c)    2. (b)    3. (d)    4. (b)    5. (c)  
 6. (a)    7. (d)    8. (b)    9. (c)    10. (c)



#### Student's Assignments

#### Explanations

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.

■■■■