

Electronics Engineering

Materials Science

Comprehensive Theory

with Solved Examples and Practice Questions



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Corporate Office: 44-A/4, Kalu Sarai (Near Hauz Khas Metro Station), New Delhi-110016

E-mail: infomep@madeeasy.in

Contact: 011-45124612, 0-9958995830, 8860378007

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Materials Science

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First Edition: 2015

Second Edition: 2016

Third Edition: 2017

Fourth Edition: 2018

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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.

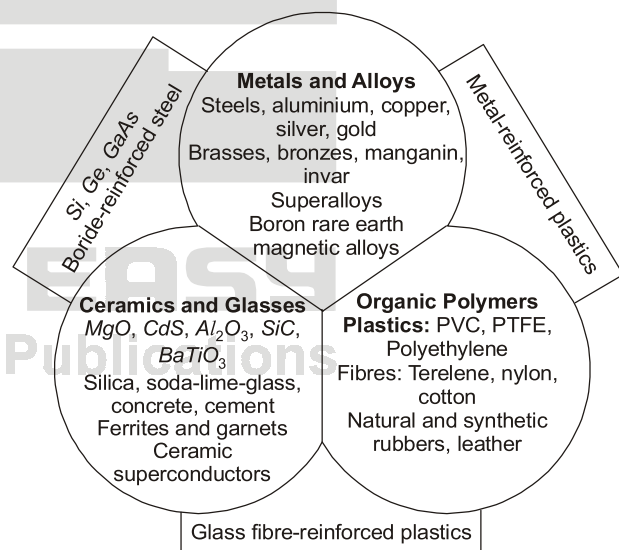
For any kind of product every engineer is vitally concerned with the materials available to him. While making a choice of material for a particular product an engineer must be aware of basic atomic structure of the materials and take into account such properties as strength, electrical conductivity, 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.



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, LaMnO₃, CdCr₂Se₄, 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 = 6.62×10^{-34} Js

c = Speed of light = 2.998×10^8 m/s

λ = 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

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.

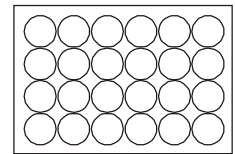
But this is not a rule. In crystalline solids the atoms are arranged in a regular geometrical array known as **space lattice**. These lattices are described by a unit building block which is essentially repeated throughout space in a periodic manner. Such blocks are known as unit cells. A crystalline 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.

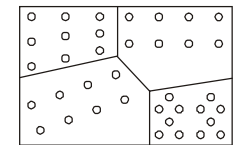
1.7.3 Single Crystal

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 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° ; \vec{a} and \vec{b} are called the **fundamental translation vectors** that generate the square array.

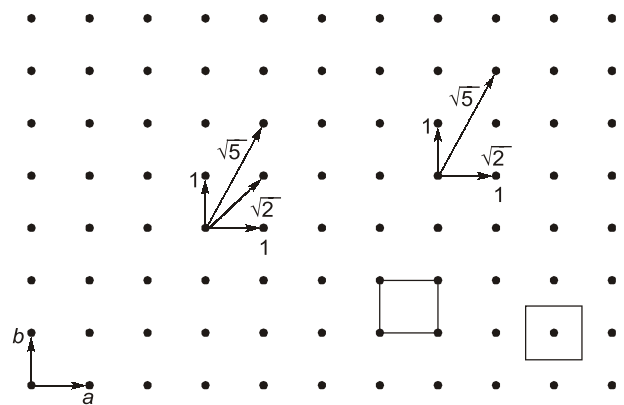
If we locate ourselves at any point in the array and look out in a particular direction that lies on the plane of the paper, the scenery is the same, irrespective of where we are. Consider the immediate surroundings of a

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.

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 combined with the basis generates a unit cell. Thus,

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

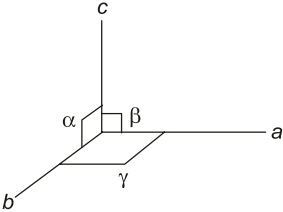
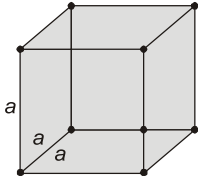
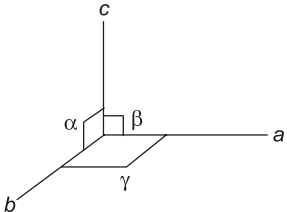
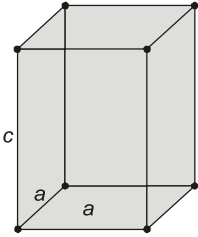


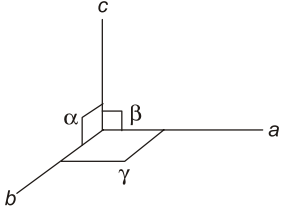
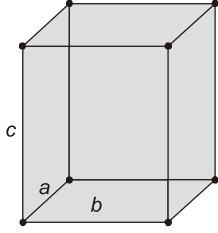
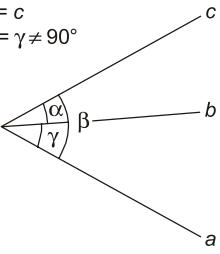
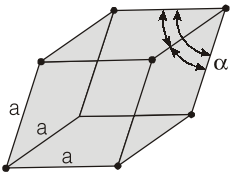
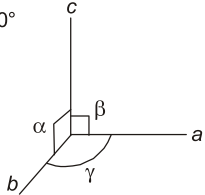
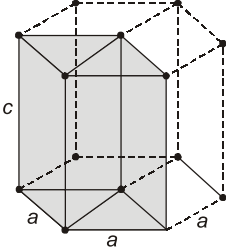
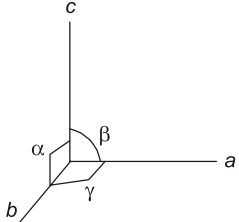
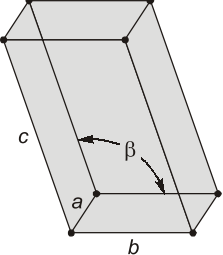
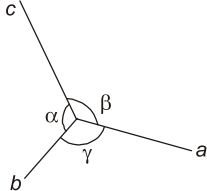
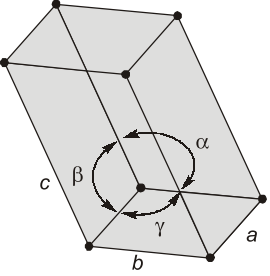
A two dimensional square array of points gives a square lattice. Two ways of choosing a unit cell are illustrated

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
<p>1. Cubic $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$</p> 	<ol style="list-style-type: none"> Simple (Lattice points at the eight corners of the unit cell). Body centred (Points at the eight corners and at the body centre). Face centred (Points at the eight corners and at the six face centres). 	
<p>2. Tetragonal $a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$</p> 	<ol style="list-style-type: none"> Simple (Points at the eight corners of the unit cell). Body centred (Points at the eight corners and at the body centre). 	

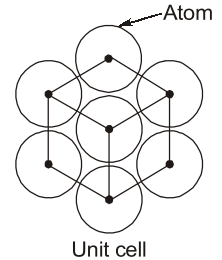
<p>3. Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$</p> 	<p>6. Simple (Points at the eight corners of the unit cell).</p> <p>7. End centred (Also called side centred or base centred) (Points at the eight corners and at two face centre opposite to each other)</p> <p>8. Body centred (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>4. Rhombohedral or Trigonal $a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$</p> 	<p>10. Simple (Points at the eight corners of the unit cell).</p>	
<p>5. Hexagonal $a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$</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>6. Monoclinic $a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$</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>7. Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$</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 di-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).

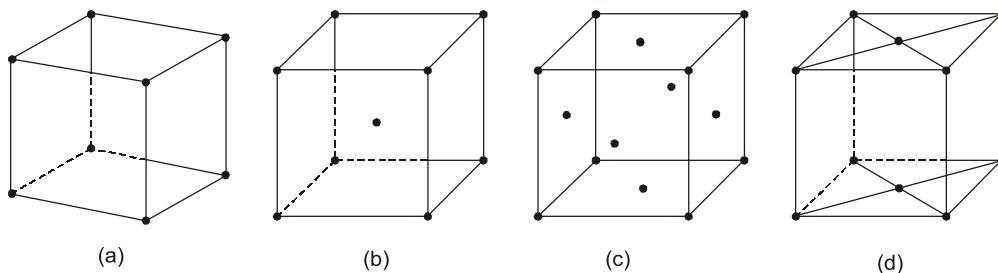
$$\text{i.e. } 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 1 + 3 = 4 \text{ lattice points/unit cell.}$$

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).

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



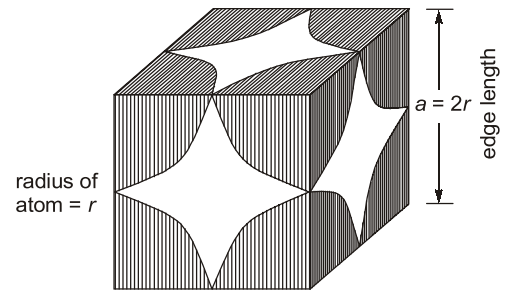
1.13 Cubic Crystal Structures

There are three cubic crystal structures:

1.13.1 Simple Cubic Crystal Structure (SCC)

In a simple cubic structure, there is one lattice point at each of the eight corners of the unit cell. If we take an atom at one corner as the centre, it is observed that this atom is surrounded by six equidistant nearest neighbours and hence the **co-ordination number of a simple cubic lattice is six**.

In this structure, each corner atom is shared by **eight unit cells**.



Simple cubic structure

Atomic Radius

Atomic radius is defined as, “**half the distance between nearest neighbours in a crystal of pure element.**”

Figure shows the unit cell of a simple cubic structure.

Let r be the radius of atom.

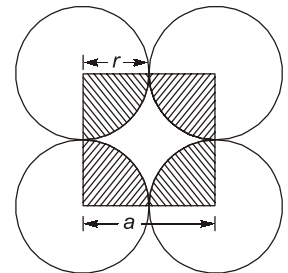
In simple cubic (SCC) lattice

$$a = 2r$$

\therefore

$$r = \frac{a}{2}$$

...(1.3)



Atomic Packing Factor

The packing of atoms in a unit cell of the crystal structure of a material is known as atomic packing factor (APF).

i.e.

$$\text{APF} = \frac{\text{Total volume of the atoms per unit cell}}{\text{Volume of the unit cell}}$$

...(1.4)

It is also known as **packing efficiency (η)**.

For simple cubic structure,

$$\text{APF} = \frac{N \times \text{volume of each sphere}}{\text{Total volume of each cell}}$$

Where, N = total number of atoms in each unit cell.

For simple cubic, **$N = 1$**

$$\text{Radius of each sphere} = r = \frac{a}{2}$$

$$\text{Volume of each sphere} = \frac{4\pi}{3} r^3 = \frac{4\pi}{3} \times \left(\frac{a^3}{8}\right) = \frac{\pi}{6} a^3$$

\therefore

$$\text{APF} = \frac{1 \times (\pi/6) a^3}{a^3} = \frac{\pi}{6} = 0.52$$

$$\% \text{ APF} = 52.4\% \text{ filled}$$

1.13.2 Body Centred Cubic Structure (BCC)

In BCC structure, in a unit cell, there are eight atoms at the eight corners and another atom at the body centre. The corner atoms do not touch each other, but each corner atom touches the body centre atom along the body diagonal as shown in figure.

Hence the co-ordination number of BCC structure is eight.

Atomic Radius of BCC

From figure,

$$AG = r + 2r + r = 4r$$

In $\triangle DCG$,

$$DG^2 = DC^2 + CG^2$$

$$DG = \sqrt{a^2 + a^2}$$

Diagonal of face = $a\sqrt{2}$

\therefore In $\triangle DGA$,

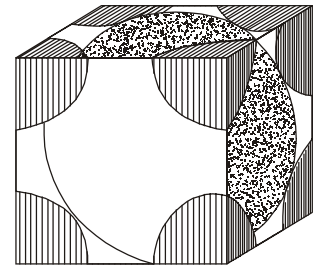
$$AG^2 = a^2 + (a\sqrt{2})^2$$

$$AG = a\sqrt{3} = \text{diagonal of cube}$$

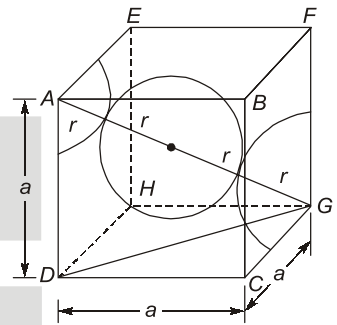
Also,

$$4r = a\sqrt{3}$$

$$r = \frac{a\sqrt{3}}{4}$$



Body centered cubic structure



...(1.5)

Atomic Packing Factor

For BCC, $N = 2$ and $r = \frac{a\sqrt{3}}{4}$

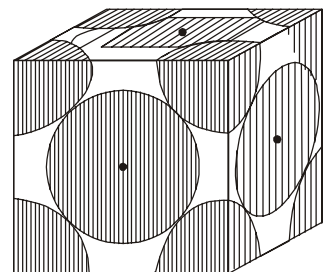
$$\text{Volume of each sphere} = \frac{4\pi}{3} r^3 = \frac{4\pi}{3} \left(\frac{a\sqrt{3}}{4} \right)^3 = \frac{\pi\sqrt{3}}{16} a^3$$

$$\text{APF} = \frac{N \times \text{Volume of each sphere}}{\text{Total volume of each cell}} = \frac{2 \times \frac{\pi\sqrt{3}}{16} a^3}{a^3} = \frac{\pi\sqrt{3}}{8} = 0.68$$

% APF = 68% filled

1.13.3 Face Centered Cubic Structure (FCC)

- In FCC structure, one atom lies at each corner of the cube in addition to one atom at the centre of each face.
- For any corner atom, there are four atoms at each corner that surround it.
- Each face centre has an atom. There are four atoms nearest to the atom on four atomic planes below it and four above it in the atomic plane.
- The co-ordination number of face centred cubic structure is thus $4 + 4 + 4 = 12$.



Face centered cubic structure

NOTE: The **co-ordination** number is defined as the number of nearest and equidistant atoms with respect to any other atom in a unit cell.

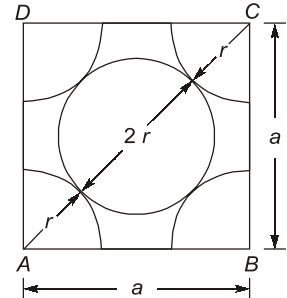
Atomic Radius of FCC

From figure,

$$\begin{aligned} AC^2 &= AB^2 + BC^2 \\ (r + 2r + r)^2 &= a^2 + a^2 \\ 16r^2 &= 2a^2 \end{aligned}$$

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

...(1.6)



Atomic Packing Factor

For FCC, $N = 4$ and $r = \frac{a\sqrt{2}}{4}$

$$\text{Volume of each sphere} = \frac{4\pi}{3} r^3 = \frac{4\pi}{3} \left(\frac{a\sqrt{2}}{4} \right)^3 = \frac{\sqrt{2}\pi}{24} a^3$$

$$\therefore \text{APF} = \frac{4 \times \frac{\sqrt{2}\pi a^3}{24}}{a^3} = \frac{\sqrt{2}\pi}{6} = \frac{\pi}{3\sqrt{2}} = 0.74$$

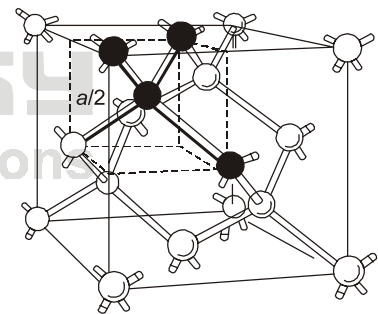
% APF = 74% filled

1.13.4 Diamond Cubic (DC) Structure

Carbon exists in two forms viz. **diamond** and **graphite**. Both have quite different characteristics and properties.

Diamond:

- ⇒ (sp^3) hybrid covalent bond.
- ⇒ Each of its atoms has four bonds.
- ⇒ The bonds are directional in nature.
- ⇒ The bonds are primary bonded and are extended in a three-dimensional network.
- ⇒ The **directional bond angle in diamond is 109.5°** .
- ⇒ The structure of diamond is better known as diamond cubic (D.C.).
- ⇒ **Graphite** is another form of carbon in which covalent bond is of (sp^2) hybrid type. There are **three bonds per atom** in it with **bond angle of 120°** .



Diamond lattice unit cell, showing the four nearest neighbour structure

Regarding diamond cubic structure, it should be noted that:

- ⇒ It consists of two inter-penetrating FCC arrangement of carbon atoms.
- ⇒ **Unit cell of DC contains 18 atoms.** Of these 8 are placed on corners of the cube, one on each of the six faces and 4 inside it i.e. $(8 + 6 + 4 = 18)$ atoms.

- ⇒ The space lattice of DC is face centered cubic (FCC).
- ⇒ There are tetrahedral co-ordination of carbon atoms.
- ⇒ Number of atoms in the DC unit cell = $\frac{1}{8} \times 8$ (corner atom) + $\frac{1}{2} \times 6$ (face centered atoms) + 1×4 (atom inside the cell) = $1 + 3 + 4 = 8$.
- ⇒ The distance of separation between the two atoms of the basis (nearest neighbours) is $= a\sqrt{\left(\frac{1}{4}-0\right)^2 + \left(\frac{1}{4}-0\right)^2 + \left(\frac{1}{4}-0\right)^2} = \frac{a\sqrt{3}}{4}$ (where a is the lattice parameter of DC unit cell).

Atomic Packing Factor of Diamond Cubic (DC) Structure

For DC, $N = 8$ and $r = \frac{a\sqrt{3}}{8}$

$$\therefore \text{APF} = \frac{8 \times \frac{4\pi}{3} \left(\frac{a\sqrt{3}}{8}\right)^3}{a^3} = \frac{\pi\sqrt{3}}{16} = 0.34$$

% APF = 34% Packed

1.13.5 Hexagonal Closed Packing

In hexagonal closed packing there are 12-atoms at 12-corners of the hexagonal, 2 atoms at the top and bottom of hexagonal and three are inside

$$\text{atom/cell} = 12 \times \frac{1}{6} + 2 \times \frac{1}{2} + 3 = 6$$

Co-ordination No. 12

APF: 0.74, Ex. Be, Cd, Co, Mg, Zn etc.

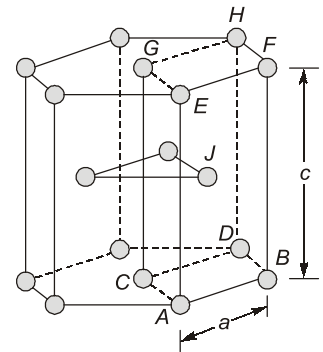


Table-1.1 for Cubic Crystal Structure

S.No.	Properties	Simple Cube (SC)	Body centered cube (BCC)	Face centered cube (FCC)	Diamond cube (DC)
1.	Volume of unit cell.	a^3	a^3	a^3	a^3
2.	No. of atoms/unit cell	1	2	4	8
3.	No. of atoms/unit volume	$\frac{1}{a^3}$	$\frac{2}{a^3}$	$\frac{4}{a^3}$	$\frac{8}{a^3}$
4.	Co-ordination No.	6	8	12	4
5.	Nearest neighbour distance (2r)	a	$\frac{a\sqrt{3}}{2}$	$\frac{a\sqrt{2}}{2}$	$\frac{a\sqrt{3}}{4}$
6.	Atomic radius	$\frac{a}{2}$	$\frac{a\sqrt{3}}{4}$	$\frac{a\sqrt{2}}{4}$	$\frac{a\sqrt{3}}{8}$
7.	Atomic packing factor	$\frac{\pi}{6} = 0.52$	$\frac{\sqrt{3}\pi}{8} = 0.68$	$\frac{\sqrt{2}\pi}{6} = 0.74$	$\frac{\pi\sqrt{3}}{16} = 0.34$
8.	Examples	Polonium, Fluorspar, Manganese	Sodium, Lithium, Chromium, Fe, Ti, Mn, K	Aluminium, Copper, Silver, Lead, Pt, Ni, Au	Germanium, Silicon and Carbon

1.14 Miller Indices

Miller indices are the styles to designate the planes and directions in the unit cells and crystals. Such designations become essential for investigations of various properties in different elements. In most general way, the Miller indices are expressed by (hkl) and no comma is used between them. Here, the symbols h , k and l indicate unknown integers. Different kinds of brackets have special meanings which are elaborated as below:

- (hkl) denotes a plane.
- $[hkl]$ denotes a direction.
- $\{hkl\}$ denotes a family of planes.
- $\langle hkl \rangle$ denotes family of directions.

Miller indices (hkl) are expressed as a reciprocal of intercepts p , q and r made by the plane on the three rectangular axes x , y and z respectively. The intercepts are measured in terms of dimensions of unit cell. These are unit distances from the origin along the three axes. Thus,

$$h = \frac{1}{p}, \quad k = \frac{1}{q} \quad \text{and} \quad l = \frac{1}{r}$$

- where, p = intercept of the plane on x -axis,
 q = intercept of the plane on y -axis, and
 r = intercept of the plane on z -axis.

Reciprocal of these intercepts are then converted into whole numbers. This can be done by multiplying each reciprocal by a number obtained after taking LCM (Lowest Common Multiplier) of denominator. This gives the Miller indices of the required plane. The Miller indices are expressed by three **smallest integers**.

1.14.1 Determining the Miller Indices of a Given Plane

Refer figure showing a plane ABC in a cubical unit cell. We have to determine Miller indices of plane ABC. Origin O and coordinate axes x , y and z are shown in the unit cell in which $OP = OQ = OR = a$. The plane in question intercepts at A , B and C on x , y and z axes in such a way that,

$$OA = \left(\frac{2a}{3}\right) \text{ along } x\text{-axis,}$$

$$OB = \left(\frac{2a}{5}\right) \text{ along } y\text{-axis,}$$

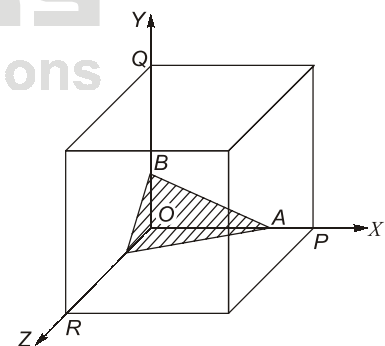
and
$$OC = \left(\frac{1a}{3}\right) \text{ along } z\text{-axis}$$

To obtain the required Miller indices, we proceed as below:

- (i) The intercepts are $C_1 = OA$, $C_2 = OB$ and $C_3 = OC$, therefore,

$$p(\text{along } x\text{-axis}) = \frac{OA}{OP} = \frac{(2/3)a}{a} = \frac{2}{3}$$

$$q(\text{along } y\text{-axis}) = \frac{OB}{OQ} = \frac{(2/5)a}{a} = \frac{2}{5}, \text{ and}$$



Determination of Miller indices of an unknown plane

$$r(\text{along } z\text{-axis}) = \frac{OC}{OR} = \frac{(1/3)a}{a} = \frac{1}{3}$$

(ii) As $h = \frac{1}{p}$, $k = \frac{1}{q}$ and $l = \frac{1}{r}$, therefore,

$$h = \frac{1}{(2/3)} = \frac{3}{2} \quad k = \frac{1}{(2/5)} = \frac{5}{2} \quad \text{and} \quad l = \frac{1}{(1/3)} = \frac{3}{1}$$

$$\therefore (hkl) = \left(\frac{3}{2} \frac{5}{2} \frac{3}{1} \right)$$

(iii) As (hkl) should have smallest possible integers, hence we can write

$$(hkl) = \frac{1}{2} (356)$$

Here the factor 1/2 is the result of conversion of reciprocals to integers, and is usually omitted.

We, therefore, conclude that Miller indices of plane ABC is

$$(hkl) = (356)$$

Miller indices of planes in non-cubical unit cells may be determined in the same manner.

1.15 Planar Density

The number of atoms per unit area of a crystal plane is known as **Planar density**. This density expresses the packing of atoms on a plane. The planar density ρ_p can be expressed as,

$$\rho_p = \frac{N_e}{A} \quad \dots(1.7)$$

where N_e is the effective number of atoms on the plane whose area is A .

⇒ Planar density in SC on (111) plane

$$\rho_p = \frac{0.58}{a^2} \quad \dots(1.8)$$

⇒ Planar density in BCC on (110) plane

$$\rho_p = \frac{1.414}{a^2} \quad \dots(1.9)$$

⇒ Planar density in Face Centred Cube (FCC) on (100) plane

$$\rho_p = \frac{2}{a^2} \quad \dots(1.10)$$

1.16 Interplanar Spacing

The spacing between a plane (hkl) and the other parallel plane passing through the origin is called interplanar spacing. It is denoted by $d_{(hkl)}$. It is measured at right angles to the planes. Interplanar spacing may be obtained from the following relations in cubic and tetragonal crystals.

For cubic unit cell,

$$d_{(hkl)} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

and for tetragonal unit cell,

$$d_{(hkl)} = \frac{1}{\sqrt{h^2 + k^2 + l^2(a^2/c^2)}}$$

Member of a family of planes (hkl) have the same interplanar spacing.

1.17 Properties of Engineering Materials

The properties of all materials arise from their structure i.e. the manner in which their atom aggregate to form molecules or crystals.

The practical application of all types of engineering materials depends upon the knowledge of their particular properties under a wide range of conditions. Some of the most important properties of the materials are:

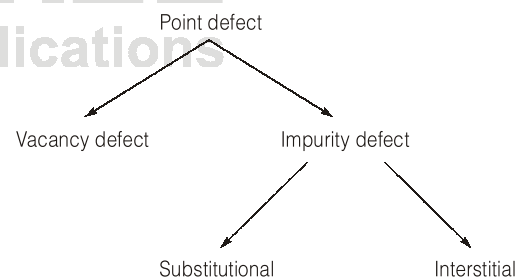
- | | |
|-------------------------|---|
| ⇒ Mechanical properties | – Strength, stiffness, elasticity, plasticity, ductility, toughness, hardness, brittleness, malleability etc. |
| ⇒ Thermal properties | – Specific heat, thermal expansion, thermal conductivity etc. |
| ⇒ Electrical properties | – Conductivity, resistivity, dielectric permeability, dielectric strength etc. |
| ⇒ Magnetic properties | – Permeability, coercive force etc. |
| ⇒ Physical properties | – Dimensions, density, porosity, structure etc. |
| ⇒ Chemical properties | – Corrosion resistance, acidity, composition, oxidation etc. |
| ⇒ Optical properties | – Colour, light transmission, light reflection etc. |
| ⇒ Acoustical properties | – Sound transmission, sound reflection etc. |

1.18 Structural Imperfections

- Point defect
- Line defect
- Surface defect
- Volume defect

1.18.1 Point Defect

Point defects are defects that occur only at or around a single lattice point. They are not extended in space in any dimension.

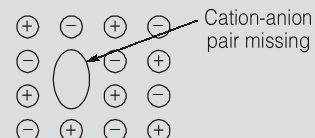


- Vacancy defect:** It is a point defect which involves a missing atom within a crystal structure.

NOTE



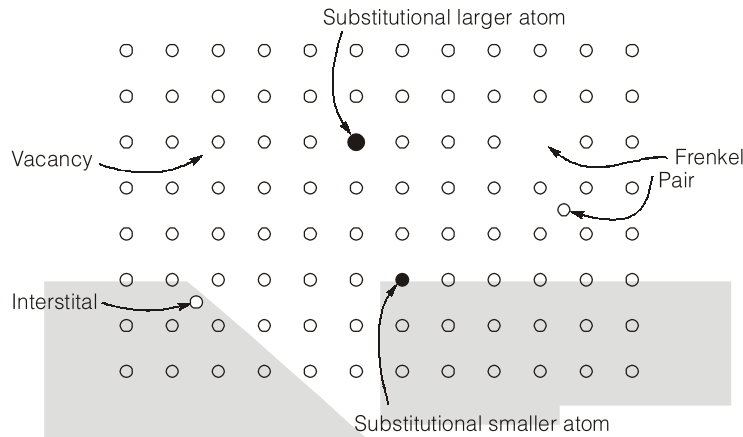
Schottky defect is a kind of vacancy defect in which cation-anion pairs are missing.



2. **Impurity defect:** It arises when a foreign atom introduced in a crystal lattice either as an interstitial or substitutional entity.

Interstitial: An interstitial impurity is a small sized atom which occupied void in the crystal structure.

Substitutional : A substitutional impurity defect refers to a foreign atom that replaces a parent atom with in crystal structure.



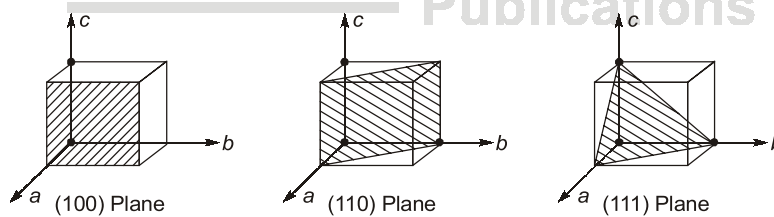
1.18.2 Line Defect

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,

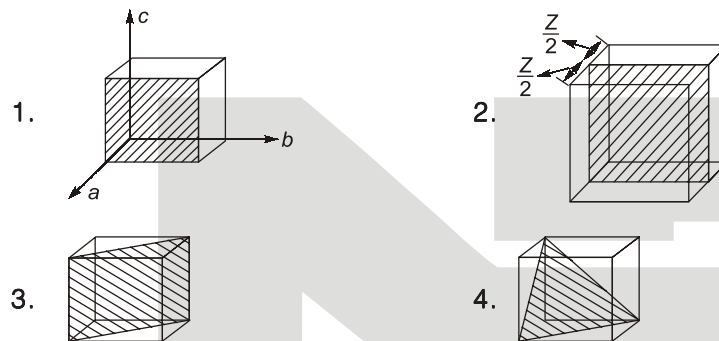
$$r = 1.06 \text{ \AA}$$

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

Inter planar separation for (111) planes is

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

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)

[IES : 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

[IES : 2009]

Ans. (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,

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