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# Crystal Physics

## (1) INTRODUCTION

There are five different states of matter namely solid, liquid, gas, plasma and Bose-Einstein condensate. Solid state is defined as that state of matter which has a fixed and definite shape at room temperature. A solid consists of atoms, molecules or ions packed closely together and the forces holding them are responsible for various distinctive properties of the solid. The bonds between constituent particles of a solid can be covalent, ionic, VanderWalls, and metallic bonds. These bonds can link an unlimited number of constituent particles to give a definite shape to the solid. All types of bonds mentioned above involve electric forces. Solids constitute very small portion of our universe but these of much interest for us because a large part of modern technology is based on the special characteristics of various solid materials.

On the basis of atomic/molecular/ionic arrangement, solids can be further classified as Crystalline and Amorphous. Crystalline solids are those, in which atoms/molecules/ions are arranged in a regular three dimensional pattern. For example quartz, calcite, rock salt, sugar, diamond etc. Amorphous solids are those in which constituent particles are arranged in irregular manner. For example Rubber, Glass, Plastic, Paraffin etc. These are also called Glassy Solids. Most of the solid matter is crystalline *i.e.* nature favours crystalline state of solids. It is because

Table 1

Crystalline Solids	Amorphous Solids
<ol style="list-style-type: none"><li>1. They exhibit long range order.</li><li>2. All bonds are of equal strength.</li><li>3. They have sharp melting points.</li><li>4. They are anisotropic <i>i.e.</i> their physical properties like mechanical strength, refractive index, electrical and thermal conductivity are different in different directions.</li></ol>	<ol style="list-style-type: none"><li>1. They do not show long range order.</li><li>2. Different bonds have different strengths.</li><li>3. They do not have sharp melting point. Instead, they have a range of temperature, in which solid sample melts completely.</li><li>4. They are isotropic <i>i.e.</i> their physical properties are same in all directions.</li></ol>

of the fact that energy of ordered atomic arrangement is lower than that of irregular packing of atoms. However when atoms are not given opportunity to arrange themselves properly (e.g. temperature of a liquid is cooled abruptly), then during solidification, no order is maintained. Hence under such condition, amorphous solids are formed. Amorphous solids can be regarded as super cooled liquids, whose stiffness or hardness is because of exceptionally high value of viscosity. This analogy is further supported by the fact that density of a given liquid is usually closer to the density of corresponding solid. Table (1) compares properties of Crystalline & Amorphous solids.

## (2) CRYSTAL

An ideal crystal is an arrangement of identical structural units repeated again and again in space and have no boundaries at all. This means the environment of every atom/molecule/ion in a crystal is identical. However in actual practice every solid substance has finite dimensions. Hence ideal crystal does not exist. In actual practice two different cases may arise.

(i) The regularity of pattern is maintained throughout a given volume of solid. In this case the complete specimen is called a single crystal. Such solids are crystalline at microscopic scale as well as macroscopic scale. Examples of single crystals (or single crystal solids) are copper, silver, gold, iron, aluminium and alkali metals. In these the structural unit is the respective atom of the element. However it should be noted that structural unit may be molecules or ions also.

(ii) The regularity of pattern is maintained upto certain volume instead of complete volume of solid piece. This portion of the solid upto which order is maintained is called grain or single crystal and the faces of single crystals are called Grain Boundaries. At grain boundary periodicity or order of arrangement is broken. In the complete piece of such a solid large number of grains (single crystals) of various shapes or sizes are packed into one another in an irregular manner. These materials are called Polycrystalline. For example ceramics and most of ionic salts are Poly crystals. If the size of grain is very large then Poly crystals show properties of crystalline solids at microscopic as well as macroscopic level. If grain size is medium then solid will show properties of crystalline substance at microscopic level. However large specimens will show properties of Amorphous solids. If grain size is itself submicroscopic i.e. very small, then solid becomes an amorphous solid.

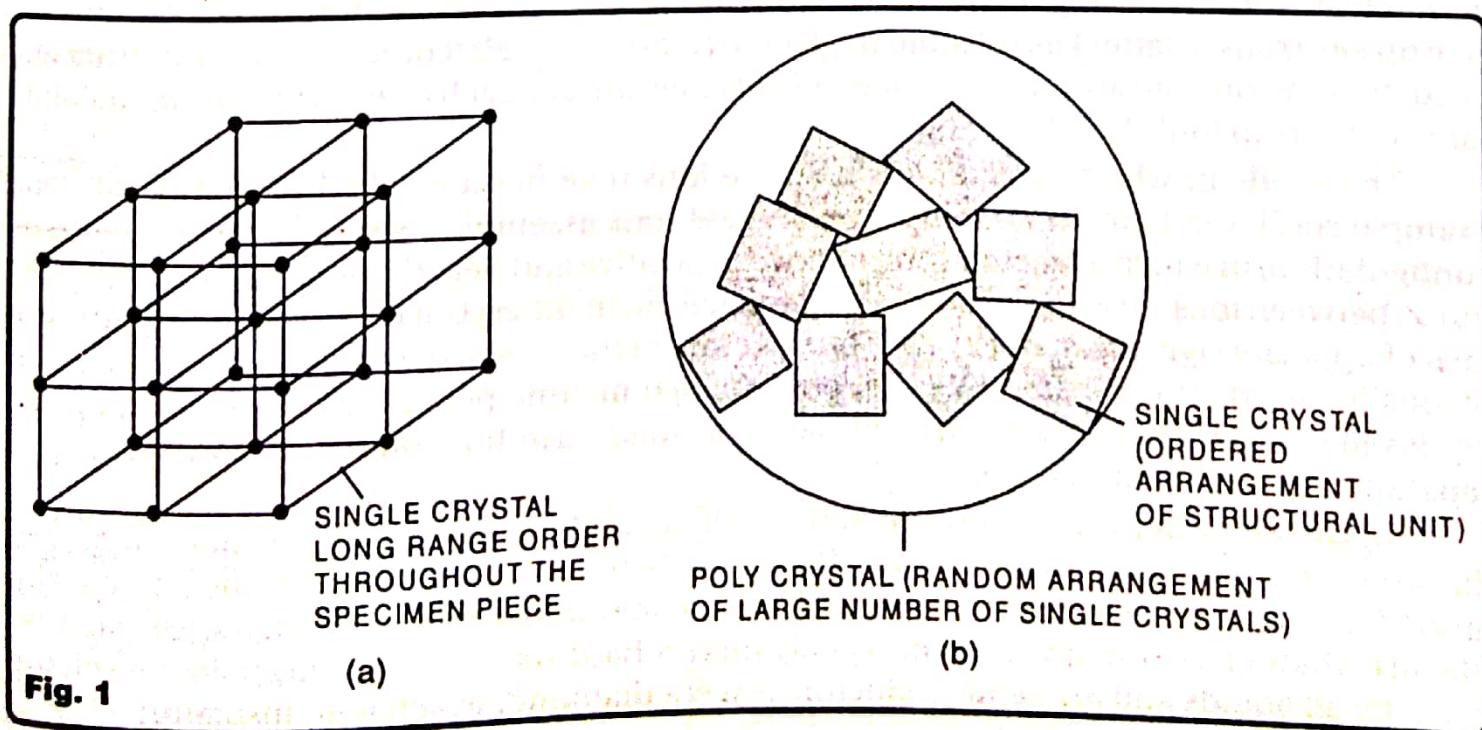


Fig. 1

### (3) COHESIVE ENERGY

"Cohesive energy of a crystalline solid is the work needed to remove an atom (or molecule) from the crystal". It indicates the strength of the bonds holding an atom in a crystal. It is also called binding energy of solid. It should be noted that atoms or molecules in a solid are more stable as compared to corresponding atoms or molecules in gaseous form. It means that total energy of a solid is less than sum of energies of free atoms or molecules. It means when a solid is formed, there is always a release in energy. Conversely if a solid is to be dissociated into atoms or molecules, then energy has to be supplied externally. This discussion allows us to find cohesive energy of a solid as follows :-

Let  $E_s$  = total energy of a solid

$N$  = total number of atoms or molecules in the solid

$E_a$  = Energy of one free atom or molecule.

$NE_a$  = total energy of free atoms or molecules

$\Delta E$  = Energy released during formation of solid

$$= NE_a - E_s$$

$E_c$  = cohesive energy = energy released per atom

$$= \frac{\Delta E}{N} = E_a - \frac{E_s}{N} \quad \dots(1)$$

Cohesive energy is usually expressed as eV/molecule and occasionally as eV/mole. The stability of a solid arises from resultant of both attractive and repulsive interactions between ions and electrons. However, the way in which electrons behave in a solid gives rise to different types of bonding. Hence depending type of bonding involved, crystalline solids can be classified into various types as described in the next section.

### (4) TYPES OF CRYSTALLINE SOLIDS

Depending upon the various kinds of bonding mechanisms, crystalline solids can be classified into five different categories.

(i) **Ionic Crystals.** Ionic bonds are formed when atoms having low ionisation energy interact with atoms having high ionisation energy. In this process the former atom (low I.E.) give up electrons to latter kind of atom (high I.E.). Hence former becomes +ve ion and latter ion becomes –ve ion. These oppositely charged ions then attract each other with strong coulomb force to form an ionic bond.

The solids in which ionic bonds hold the ions together are called Ionic Crystals. For example NaCl, CsCl etc. In an ionic crystal, these ions assemble themselves in equilibrium configuration, in which attractive forces between positive and negative ions balance repulsive forces between ions. To get maximum stability each ion in the crystal is surrounded by as many ions of opposite sign as can fit closely. The structure of the crystal depends on the relative size of ions involved. These solids are hard, possess high melting point, may be soluble in polar liquids like water. These are electric insulators in solid form but conduct in solution due to separation of ions on dissolving.

(ii) **Covalent Crystals.** These are the crystalline solids in which the ionisation energies of the atoms forming the crystal are equal. Thus bond between two adjacent atoms is formed by mutual sharing of one electron from each of them. For example diamond, silicon, germanium, silicon carbide etc. Normally covalent crystals are very hard, have high melting points, insoluble in nearly all liquids and are semiconductors (except diamond, which is an insulator).

**(iii) Metallic Crystals.** The outer electrons of metal atoms are weakly bound. When such atoms interact to form a solid, their valence electrons form a gas of electrons, that move freely through the resulting assembly of metal ions (called ion core). The electron gas is responsible to hold the ions together and also provides high values of thermal and electrical conductivity, high opacity, surface lustre etc. Because the free electrons do not belong to particular atom, hence different metals can be alloyed together if their atoms are similar in size. In case of metals, the average distance of electron from an ion is less than what it would have been in case of isolated atom. Hence electron's potential energy is less in the crystal than in atom. Metallic bonds are formed when decrease in potential energy of electrons is more than increase in kinetic energy of electrons. Further the kinetic energy of electrons is more when number of valence electrons per atom are more. Due to this reason, nearly all metallic crystals or elements are found in first three groups of periodic table. Some examples of metallic crystals are sodium, gold, silver, iron etc.

**(iv) Molecular Crystals.** Molecular crystals are composed of atoms or molecules, which have no tendency to lose or even share their valence electrons with other molecules. These are the crystals of solidified gases such as  $O_2$ ,  $N_2$ ,  $H_2$ ,  $CH_4$  etc. The binding in these crystals arise from unsymmetric distribution of charge between the molecules of the crystal. When such molecule is brought together, then one molecule acquires dipole moment due to presence of other molecules around it. This interaction is attractive and is capable of binding the molecules in a crystal. Such kind of short range forces that arise due to dipole interaction (because of unsymmetric distribution of charge) are called Vander Waal's Forces. Such crystalline solids are soft, flaky, have lowest melting points, possess close packed structures and have low electrical and thermal conductivity and are usually transparent.

**(v) Hydrogen Bonded Crystals.** Hydrogen bonding occurs between certain molecules containing hydrogen atoms. The heavier atom in the molecule has more electron affinity as compared to hydrogen atom. Hence the only electron of hydrogen atom is shifted towards heavy atom and in most of cases it gets dissociated from hydrogen atom. This results in the formation of a polar molecule where positive and negative charges are separated from each other. When a large number of similar molecules are brought together, then positive charge of one molecule can link up with negative charge of other molecule. In this way a large number of molecules are held closely by strong Vander Waal's force and this type of bonding is called hydrogen bonding. Examples of Hydrogen bonded crystals are ice,  $HF_2$ ,  $KH_2PO_3$  etc. These crystals have moderately weak binding, possess loose structure, low thermal and electrical conductivity. They are transparent and possess dielectric properties. The cohesive energy of different crystal types mentioned above increases in the following fashion.

Vander Waal's < Hydrogen bonded < metallic < ionic < covalent.

## (5) CRYSTAL LATTICE AND TRANSLATION VECTORS

A crystal lattice or space lattice is an infinite repetition of points in space and each lattice point has identical surroundings. A crystal lattice is an important concept to describe crystal structure. When a group of atoms is attached to every lattice point, then we can get actual crystal structure of the solid. "The group of atoms attached to each lattice point is called Basis." Number of atoms in basis can be one, two or even more than that (can be several thousands). From above discussion we conclude that crystal structure can be completely known by the knowledge of lattice and basis and the logical relation is

$$\text{lattice} + \text{basis} = \text{crystal structure.}$$

...(2)

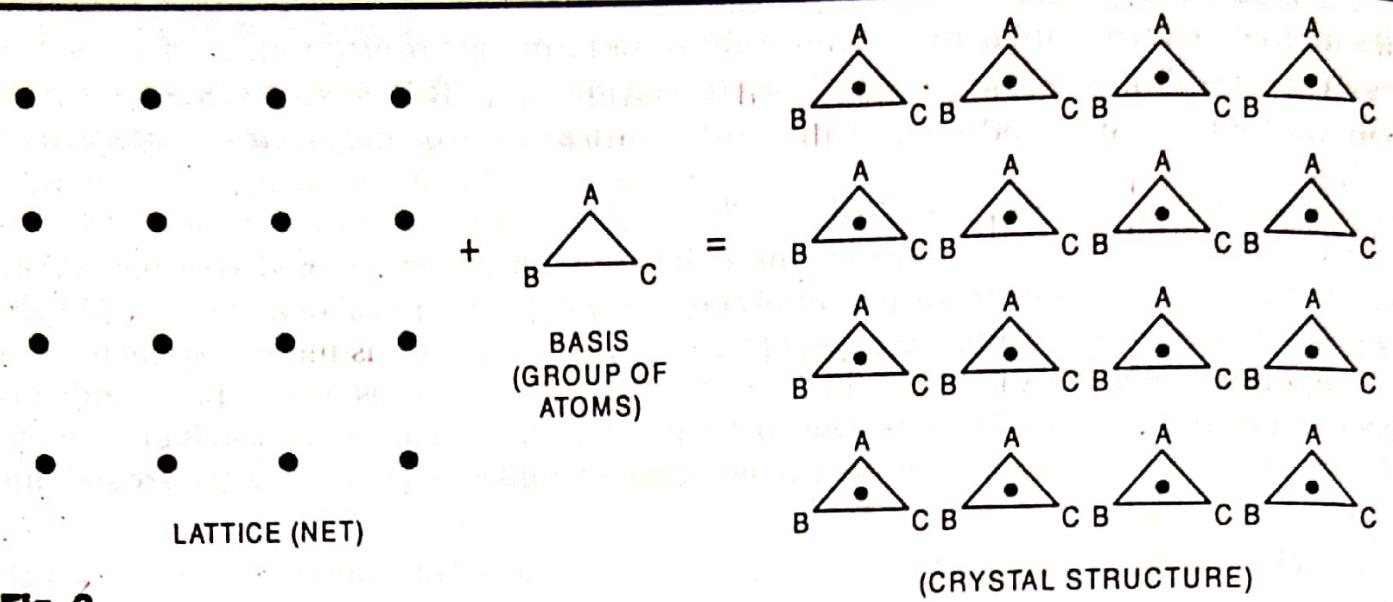


Fig. 2.

A lattice described in two dimensions is called "Net". An illustration of formation of two dimensional crystal structure from knowledge of basis and lattice is shown in fig. (2). Importance of concept of space lattice comes from the fact that we can deal with lattice points only while studying various properties of the crystal (like lattice points can be shown as diffraction centres while studying Bragg's reflection from the crystal).

A lattice is described by three fundamental translational vectors  $\vec{a}, \vec{b}, \vec{c}$ . These vectors are defined in such a way that they are non co-Planar and position of any other lattice point with respect to a reference lattice point (chosen as origin) can be described by vector addition of integral multiples of  $\vec{a}, \vec{b}, \vec{c}$ .

For example in fig. (3) we have space lattice having Fundamental Lattice Translation Vectors as  $\vec{a}, \vec{b}, \vec{c}$ . The position of a particular lattice point P is given as  $\vec{OP} = \vec{OA} + \vec{AB} + \vec{BP} = 2\vec{a} + 2\vec{c} + 1\vec{b}$  which is obeying the condition described above.

A Lattice Translation Vector of a lattice point is the position vector of that lattice point with respect to reference lattice point. It is denoted by  $\vec{T}$  and is always equal to vector sum of integral multiples of fundamental translation vectors  $\vec{a}, \vec{b}, \vec{c}$ .

$$\text{That is } \vec{T} = m\vec{a} + n\vec{b} + l\vec{c}$$

...(3)

where  $m, n, l$  are integers. Their value is different for different lattice points.

It should be noted that for a given crystal structure, more than one lattices are possible and for a given lattice, more than one set of fundamental translation vectors is possible. Once above two choices are made then basis is identified.

(i) **Unit Cell.** Consider space lattice shown in fig. (3). Here three fundamental translation vectors  $\vec{a}, \vec{b}, \vec{c}$  form a parallelopiped ODEFHIJ. It is easy to understand that if a large number of such parallelopiped units are arranged in space then space lattice is formed and if there is

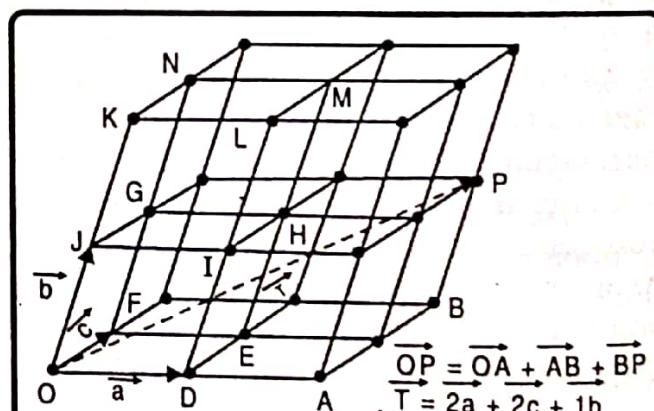


Fig. 3.

basis attached to every lattice point, then arrangement of such parallelopiped units in space will lead to crystal structure. We call this parallelopiped as unit cell.

"Hence a unit cell is a parallelopiped formed by fundamental translation vectors and when unit cells are arranged in space then space lattice or crystal structure is obtained."

However choice of fundamental translation vectors is not unique. This means, for a given lattice, more than one kinds of unit cells are possible. For example in fig. (3) we can choose  $\vec{OD}$ ,  $\vec{OF}$  and  $\vec{OK}$  as fundamental translation vectors. In this case parallelopiped ODEFNMLK will be a unit cell for the same lattice.

(ii) **Primitive Unit Cell.** A unit cell is said to be primitive unit cell if it is of smallest volume amongst all possible unit cells for a given lattice. Obviously it will contain minimum possible number of lattice points that is only one lattice point per primitive cell. In fig. (3), Parallelopiped ODEFGHIJ is a primitive unit cell while parallelopiped ODEFNMLK is non-primitive unit cell. The lengths of  $\vec{a}$ ,  $\vec{b}$ ,  $\vec{c}$  in primitive unit cell are minimum and these are denoted by  $a$ ,  $b$ ,  $c$ . These lengths are called "lattice constants" or "Primitives".

The volume of unit cell is equal to scalar triple product of fundamental translation vectors.

$$\Rightarrow V_c = \left| \vec{a} \cdot (\vec{b} \times \vec{c}) \right| \quad \dots(4)$$

(iii) **Crystallographic Axes and Interfacial Angles.** "The lines drawn along fundamental translation vectors of a primitive unit cell are called Crystallographic Axes." These are denoted as OA-axis, OB-axis, OC-axis. (Do not identify these as X, Y, Z axis because the crystallographic axes may or may not be mutually perpendicular. However these are always non-coplanar). This is shown in figure (4).

"The angles between three crystallographic axes are called interfacial angles." Angle between OA & OB axes is denoted by  $\gamma$ . The angle between OA & OC axes by  $\beta$  and angle between OB and OC axis is denoted by  $\alpha$ .

(iv) **Wigner Seitz Cell.** A Wigner Seitz cell is also a primitive cell obtained by following a special procedure as under:

(a) Draw lines to connect a given lattice point to all nearby lattice points.

(b) Draw perpendicular bisectors of each line (in 2 dimensions). In three dimensions draw normal planes at mid point of each of these lines. Then smallest volume enclosed by these planes is Wigner Seitz Primitive Cell. This is illustrated in Fig. (5).

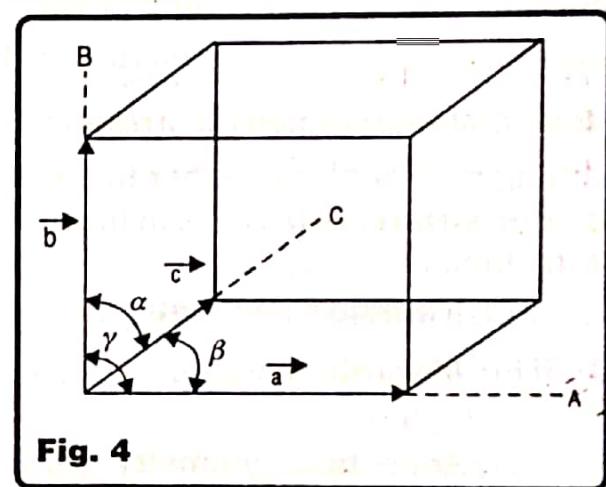


Fig. 4

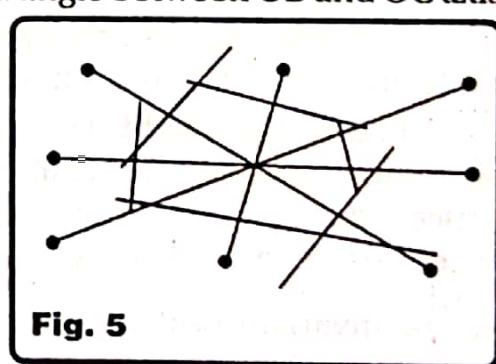


Fig. 5

## (6) CRYSTAL SYSTEMS

For discussing various possible crystal systems, we need to learn about symmetry operations.

(a) **Symmetry Operations.** "A symmetry operation is that, which when performed on the crystal structure, leaves it unchanged."

A few symmetry operations are discussed below :

(i) **Translation Symmetry.** In this operation every lattice point of crystal is translated by a constant vector. e.g. Let  $\vec{r}$  = original position of a lattice point. Let it is translated by  $\vec{T}$ , then new position of lattice point will be

$$\vec{r}' = \vec{r} + \vec{T} \quad \dots(5)$$

Since this operation is performed on all lattice points. Hence all lattice points will be displaced to their new positions after operation and new positions will be given according to equation (5). If the crystal structure after performing this operation is identical to one before applying the operation, then crystal is said to possess translational symmetry.

(ii) **Rotation Symmetry.** In this operation the crystal is rotated about an axis (passing through a lattice point) by angle  $\theta = \frac{2\pi}{n}$  (where  $n$  is a positive integer and angle  $\theta$  is expressed in radian). If this operation leaves crystal structure unchanged (invariant), then crystal is said to possess  $n$  fold rotation symmetry. Lattices can be found such that one, two, three, four and six fold rotations (corresponding to angle of rotation  $\frac{2\pi}{1}, \frac{2\pi}{2}, \frac{2\pi}{3}, \frac{2\pi}{4}, \frac{2\pi}{6}$  and integral multiples of these) leave the crystal structure unchanged. However no lattice can be found, which possess 5 fold rotation symmetry (corresponding to rotation angle  $\frac{2\pi}{5}$ ). This is because of the fact that pentagons do not fit together to fill all space. Similarly no lattice can be found having 7 fold rotation symmetry because in this case septagons cannot form unit cells, as they overlap with each other.

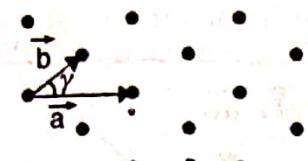
(iii) **Inversion Symmetry.** A crystal possesses an inversion symmetry, if for every lattice point having position vector  $\vec{r}$ , there is a lattice point at position  $-\vec{r}$ . For example a cube has inversion symmetry.

(iv) **Reflection Symmetry.** The reflection symmetry is symmetry of crystal about a plane passing through a lattice point. The plane of symmetry divides the crystal into two equal portions. If one portion is put on a mirror, the image will produce other half of the crystal.

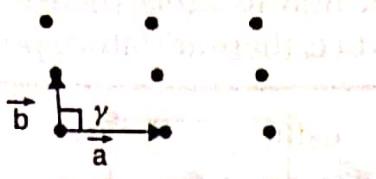
(v) **Rotation Inversion Symmetry.** A crystal is said to possess rotation inversion symmetry, if it brings out self coincidence by a rotation followed by an inversion across the centre.

(b) **Bravais Lattice.** There is an unlimited number of possible lattices because there is no restriction on value of  $a, b, c$  and angles  $\alpha, \beta, \gamma$ . In two dimensions, the general lattice is oblique lattice (See Fig. (6)(a)). This lattice is invariant only under rotation of  $\pi$  and  $2\pi$  about any axis, which passes through a lattice point. But for some specific values of  $a, b$ , and  $c$ , the 2-D lattice can be invariant under rotation of  $\frac{2\pi}{3}, \frac{2\pi}{4}$  and  $\frac{2\pi}{6}$  and mirror reflection. There are four different conditions or restrictions on the values of  $a, b, c$  so that lattice obeys a few of the above mentioned symmetry operations. This gives to 4 new special lattice types in two dimensions in addition to oblique lattice. "A lattice which shows one or more symmetry operation invariance is called Bravais Lattice". Thus in two dimensions there are five different types of Bravais Lattices (including oblique lattice).

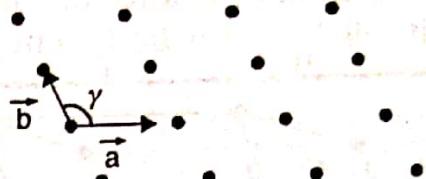
In three dimensions, the point symmetry groups require 14 different conditions on  $a, b, c, \alpha, \beta, \gamma$ . Hence we get 14 kinds of Bravais Lattices in three dimensions. The general lattice is triclinic and there are 13 other special lattices. For convenience, these are grouped in seven categories according to seven types of unit cells which are triclinic, monoclinic, orthorhombic, tetragonal, cubic, trigonal and hexagonal. These are described in table (2) below :



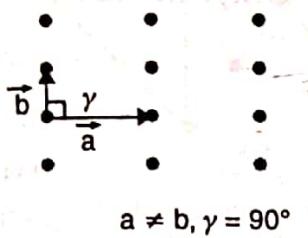
$a \neq b, \gamma \neq 90^\circ$   
(OBLIQUE LATTICE)  
(a)



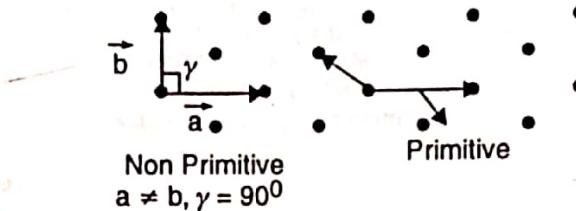
$a = b, \gamma = 90^\circ$   
(SQUARE LATTICE)  
(b)



$a = b, \gamma = 120^\circ$   
(HEXAGONAL LATTICE)  
(c)



$a \neq b, \gamma = 90^\circ$   
(RECTANGULAR LATTICE)  
(d)



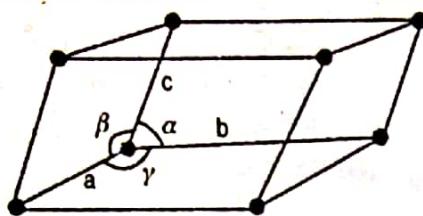
Non Primitive  
 $a \neq b, \gamma = 90^\circ$   
(CENTERED RECTANGULAR LATTICE)  
(e)

Fig. (6)

Table 2

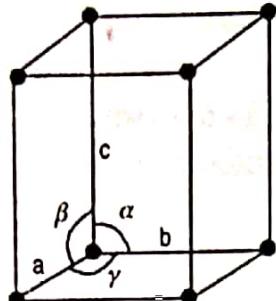
Crystal System	Bravais Lattice	Symmetry Elements	Unit cell characteristics
Triclinic	1. Simple	None	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$ .
Monoclinic	1. Simple 2. Base centered	Two Fold Rotation Axis	$a \neq b \neq c$ $\alpha \neq \beta = 90^\circ \neq \gamma$
Orthorhombic	1. Simple 2. Base centered 3. Body centered 4. Face centered	Three mutually perpendicular 2 fold rotation axes	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
Tetragonal	1. Simple 2. Body centered	One 4-fold axis and 2 two fold axes normal to 4 fold axis	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$ Right square (prism)
Cubic	1. Simple 2. Body Centered 3. Face Centered	Four 3-Fold Rotation Axes	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$
Hexagonal	1. Simple	One six fold Rotation Axis	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$
Trigonal	1. Simple	One 3-fold Rotation Axis	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$ But $\alpha, \beta, \gamma < 120^\circ$

It should be noted that in simple Bravais lattice there is one lattice point at every corner of unit cell. In case of body centered lattice, there are lattice points at each corner and one lattice



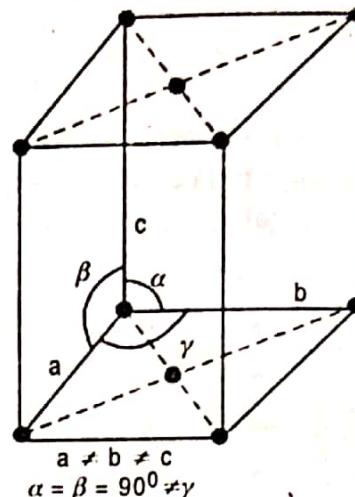
$a \neq b \neq c$   
 $\alpha \neq \beta = \gamma$   
Triclinic (Simple)  
Unit cell = Primitive  
No. of lattice points  
per unit cell =  $8 \times \frac{1}{8} = 1$

(a)



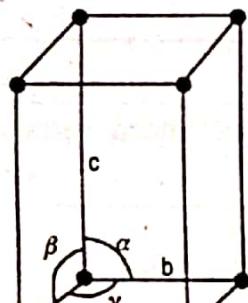
$a \neq b \neq c$   
 $\alpha = \beta = 90^\circ \neq \gamma$   
Monoclinic (Simple)  
Unit cell = Primitive  
Lattice points per unit cell = 1

(b)



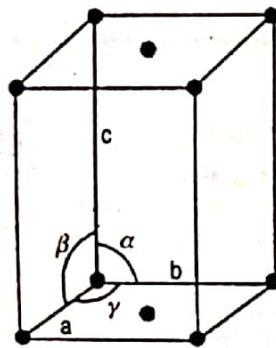
$a \neq b \neq c$   
 $\alpha = \beta = 90^\circ \neq \gamma$   
Monoclinic (Base centered)  
Unit cell = non Primitive  
Lattice Points =  $8 \times \frac{1}{8} + 2 \times \frac{1}{2} = 2$

(c)



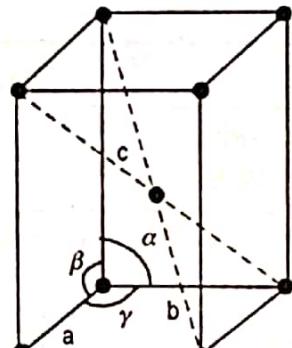
$a \neq b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$   
Orthorhombic (Simple)  
Unit cell = Primitive  
Lattice Points = 1

(d)



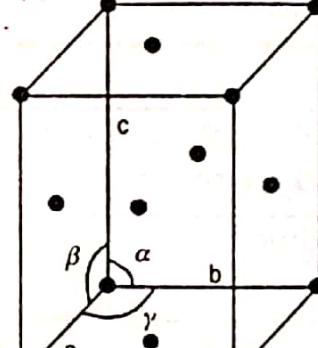
$a \neq b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$   
Orthorhombic (base centered)  
Unit cell = non primitive  
Lattice points = 2

(e)



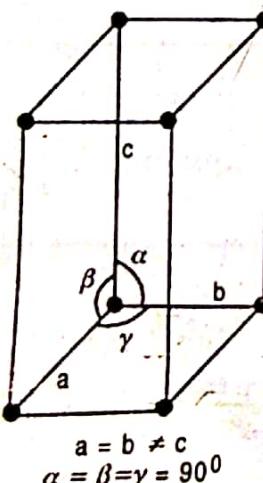
$a \neq b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$   
Orthorhombic (Body centered)  
Unit cell = non primitive  
Lattice points = 2

(f)



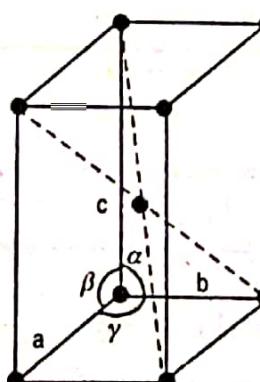
$a \neq b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$   
Orthorhombic (face centered)  
Unit cell = non primitive  
Lattice Points =  $8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$

(g)



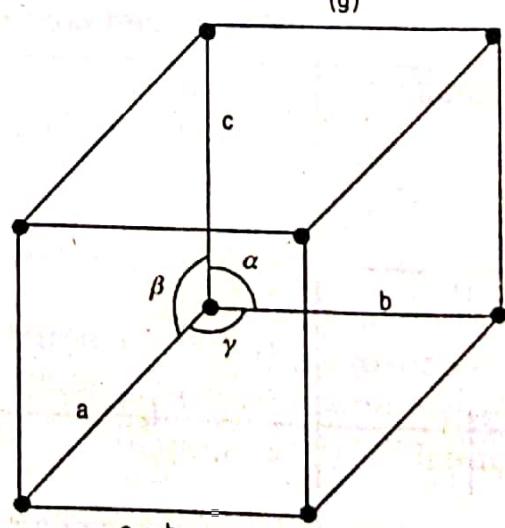
$a = b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$   
Tetragonal (Simple)  
Unit Cell = Primitive  
Lattice Points = 1

(h)



$a = b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$   
Tetragonal (body centered)  
Unit cell = non primitive  
Lattice Points = 2

(i)



$a = b = c$   
 $\alpha = \beta = \gamma = 90^\circ$   
Cubic (Simple) Unit cell = primitive  
Lattice Points = 1

(j)

**Cotd. Fig. (7).....**

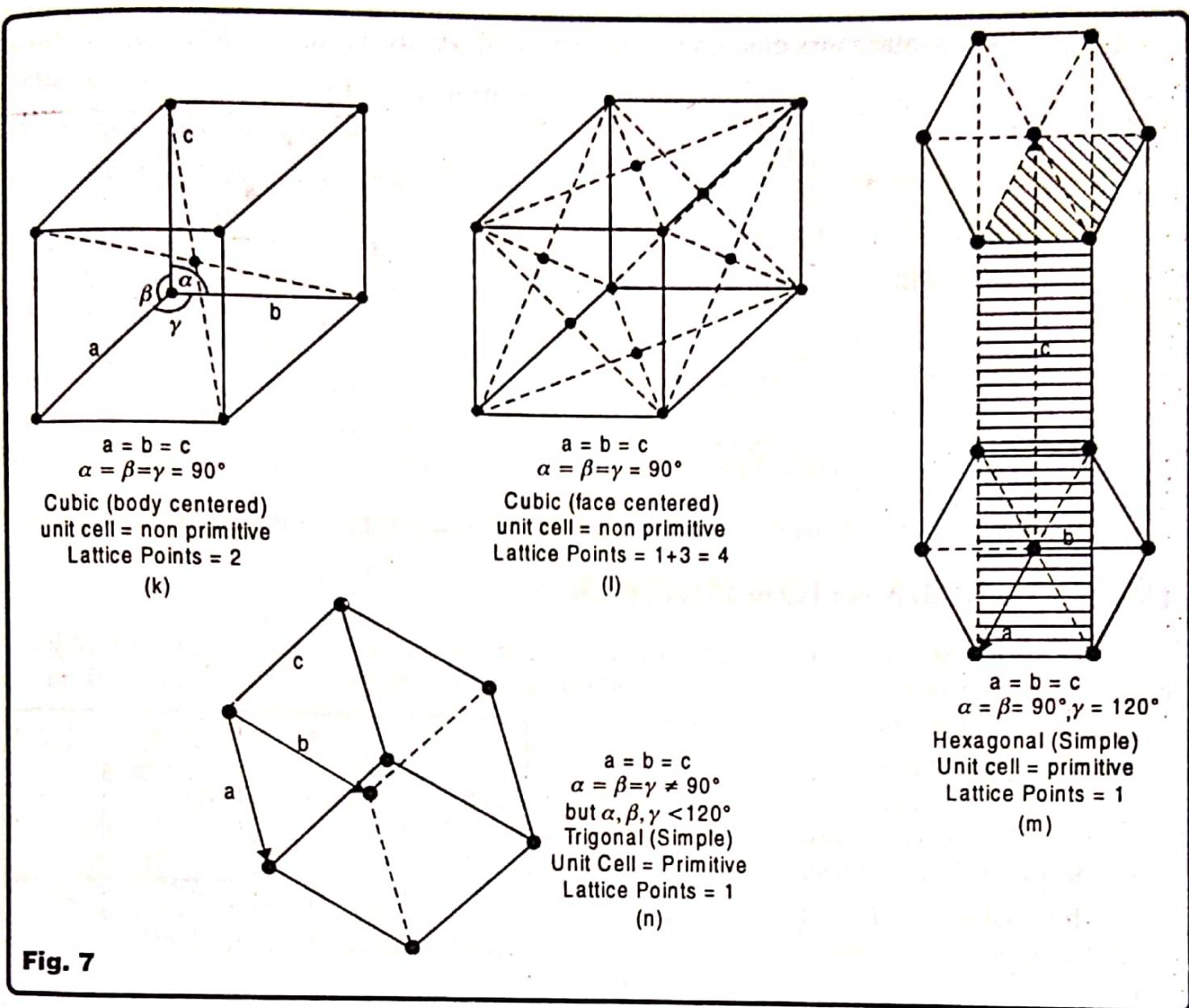


Fig. 7

point at the centre of cell. In face centered Bravais Lattice, there is a lattice point at each corner of cell and a lattice point at centre of each face of unit cell. In base centered lattice, there is a lattice point at each corner of unit cell and one lattice point at the centre of base and top face of unit cell. Keeping this in mind all 14 Bravais lattices are shown in fig. (7).

It should be noted that a lattice point at that corner of unit cell can be simultaneously shared by 8 unit cells. Hence its contribution to one particular unit cell is only  $\frac{1}{8}$ . Further a lattice point at the centre of a face can be shared by two unit cells at a time. Thus its contribution to one particular unit cell is  $\frac{1}{2}$ . However a lattice at the centre of unit cell is completely contained by it and cannot be shared by any other unit cell. Hence its contribution to unit cell is 1.

## (7) RELATION BETWEEN LATTICE CONSTANT AND DENSITY FOR CUBIC LATTICE

For a cubic lattice

$$b = c = a$$

Let  $N$  = number of molecules in the unit cell

$N_A$  = Avogadro number

... (6)

**M = Molar mass of solid**

$$\text{Mass of one molecule} = \frac{M}{N_A}$$

$$\text{Mass of unit cell } m = \frac{NM}{N_A}$$

$$\text{Volume of cubic unit cell } V = a^3$$

$$\text{Density of solid } \rho = \frac{\text{mass}}{\text{volume}} = \frac{m}{a^3}$$

$$= \frac{NM}{N_A a^3}$$

$$\Rightarrow a = \left( \frac{NM}{\rho N_A} \right)^{\frac{1}{3}}$$

...(7)

This equation can be used to calculate the lattice constant of a cubic lattice.

## (8) CO-ORDINATION NUMBER

— “The number of nearest neighbours of a lattice point in a Bravais lattice are called its co-ordination number”. It is a characteristic feature of a lattice. We shall now find out co-ordination number for a few lattice types :

(i) **Simple Cubic.** Fig. (8) shows a simple cubic lattice. Consider a lattice point O at the corner of unit cell. The nearest neighbours of this lattice point are 6 in number as shown in fig. (8).

The distance of each of these nearest neighbour from O is ‘ $a$ ’, where ‘ $a$ ’ is lattice constant. Out of the six nearest neighbours, four lie in one plane and two lie in a plane normal to it.

(ii) **Body centered cubic.** Consider a lattice point A on the corner of the unit cell. Let ‘ $a$ ’ is lattice constant. Hence distance of lattice point A from lattice points H, B and D is given as  $AB = AD = AH = a$ . Also  $AG = AC = AE = \sqrt{2} a$  (verify it)

Further it can be easily verified that

$$AF = \sqrt{3} a$$

Now O is a lattice point at the centre of unit cell. Its distance from lattice point A is  $AO = \frac{\sqrt{3}}{2} a$ . From all distances mentioned above we see that smallest distance is  $AO$ . Hence to a point at corner, the nearest neighbour is a point at the centre of unit cell and nearest neighbour separation is  $\frac{\sqrt{3}}{2} a$ . Since one corner atom is shared by eight unit cells (See Fig. (8)). Hence for every corner atom there are eight nearest neighbours at distance  $\frac{\sqrt{3}}{2} a$ . This means that co-

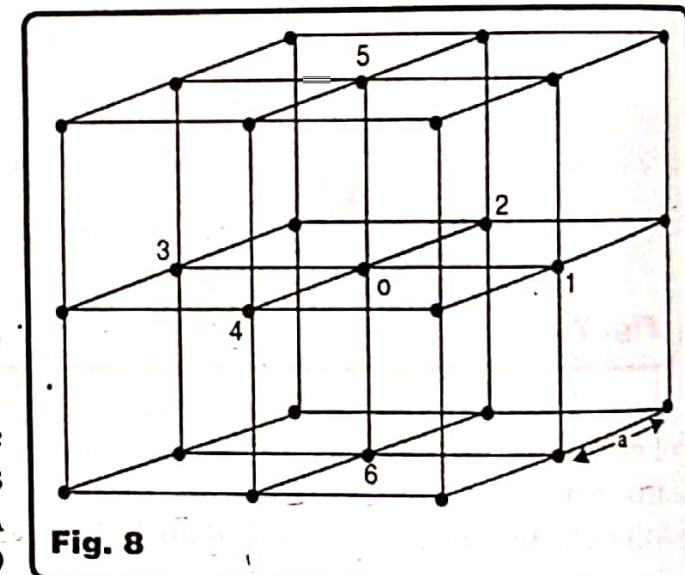


Fig. 8

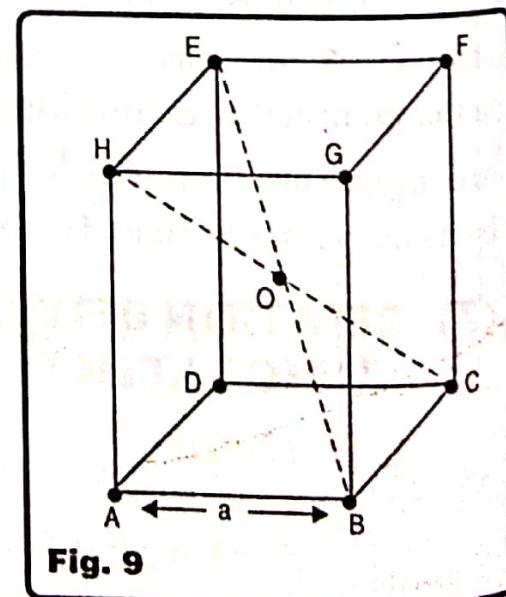


Fig. 9

## Crystal Physics

ordination number is 8. Alternatively we can consider central atom of a unit cell at point O [fig. (9)] and we see that all corner points are its nearest neighbours at separation  $\frac{\sqrt{3}}{2} a$ . Hence co-ordination number is eight.

(iii) **Face centered cubic.** Fig. (10) shows eight adjacent simple cubes of fcc lattice. For avoiding complexity of figure, Lattice points are not shown except the one at point 'O' which is shared by all eight cubes and one mentioned as no. 4. However it should be kept in mind that there is a lattice point at each corner and at centre of each face of the cube. The lattice points around O are either similar to points like P or to points like D or to points like no. 4 or points like Q. If  $a$  is lattice constant then we can easily verify that  $OP = a$  and  $OD = \sqrt{2}a$  and  $OQ = \sqrt{3}a$ .

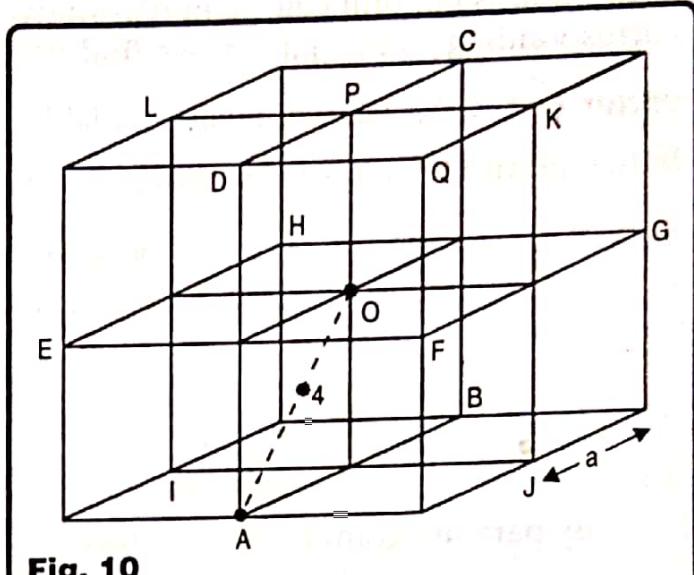


Fig. 10

However distance of point no. 4 from O is  $\frac{OA}{2} = \frac{\sqrt{2}a}{2} = \frac{a}{\sqrt{2}}$ . Out of all these distance mentioned above,  $\frac{a}{\sqrt{2}}$  is smallest. Hence points similar to no. 4 are nearest neighbours of each corner atom and having distance  $\frac{a}{\sqrt{2}}$  from it. We have shown three mutually perpendicular planes ABCD, EFGH and IJKL, all of which pass through corner point O. In each of these planes there are four nearest neighbours of point O at separation  $\frac{a}{\sqrt{2}}$ . This can be more easily understood from fig (11). Hence total number of nearest neighbours to point O are  $4 + 4 + 4 = 12$  having nearest neighbour separation  $\frac{a}{\sqrt{2}}$ .

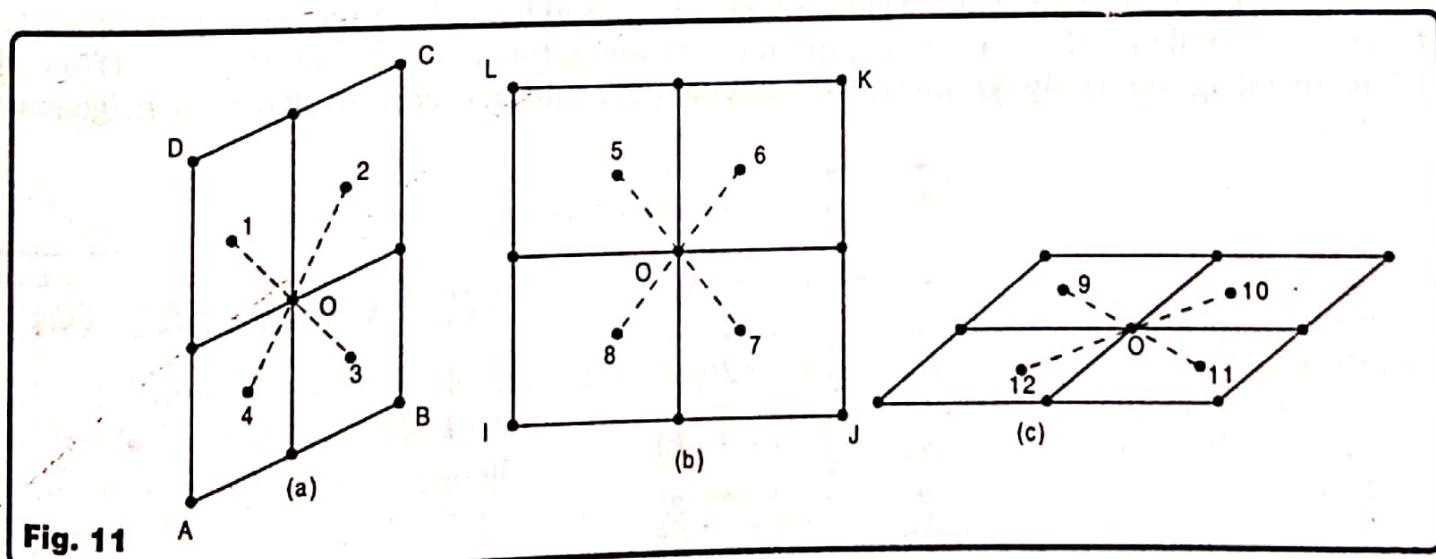


Fig. 11

## (9) VOLUME OF PRIMITIVE CELL FOR CUBIC LATTICE

(i) **Simple Cubic.** In this case the primitive lattice is a cube having lattice point at each corner of cube [See fig. (7) (j)]. If ' $a$ ' is lattice constant, then volume of primitive unit cell is  $a^3$ .

(ii) **Body centered cubic.** A bcc unit cell is shown in fig. (12). For simplicity we have shown lattice point at the centre of face OPQR only but it should be kept in mind that there is

lattice point at centre of each face. This is non-primitive unit cell as it contains  $8 \times \frac{1}{8} + 1 = 2$  lattice points per unit cell. To find primitive cell corresponding to bcc lattice, we find position vector  $\vec{OM} = \vec{A}_1$  (say) of nearest neighbour of lattice point O. We take  $\vec{OP}$  along X-axis,  $\vec{OR}$  along Y-axis and  $\vec{OV}$  along Z-axis (because lattice is cubic). Hence if  $a$  is lattice constant, then

$$\vec{OP} = a\hat{i}$$

$$\text{and } \vec{OR} = a\hat{j}$$

$$\text{and } \vec{OV} = \vec{QT} = a\hat{k}$$

By parallelogram law of vectors

$$\vec{OQ} = \vec{OP} + \vec{OR} = a(\hat{i} + \hat{j}) \quad \dots(8)$$

$$\therefore \vec{ON} = \frac{\vec{OQ}}{2} = \frac{a}{2}(\hat{i} + \hat{j}) \quad \dots(9)$$

$$\text{Also } \vec{NM} = \frac{\vec{QT}}{2} = \frac{a\hat{k}}{2} \quad \dots(10)$$

Thus by triangle law of vectors

$$\begin{aligned} \vec{OM} &= \vec{ON} + \vec{NM} \\ \Rightarrow \vec{A}_1 &= \frac{a}{2}(\hat{i} + \hat{j} + \hat{k}) \end{aligned} \quad \dots(11)$$

Since corner point O can be simultaneously shared by eight cubes. Hence like point M, there are in total of eight nearest neighbours. We want to find two more vectors from O toward its nearest neighbours. By symmetry we can write the position vectors of all nearest neighbours of O as

$$\vec{A}_2 = \frac{a}{2}(-\hat{i} - \hat{j} - \hat{k})$$

$$\vec{A}_3 = \frac{a}{2}(\hat{i} - \hat{j} - \hat{k})$$

$$\vec{A}_4 = \frac{a}{2}(-\hat{i} + \hat{j} - \hat{k})$$

$$\vec{A}_5 = \frac{a}{2}(-\hat{i} - \hat{j} + \hat{k})$$

$$\vec{A}_6 = \frac{a}{2}(-\hat{i} + \hat{j} + \hat{k})$$

$$\vec{A}_7 = \frac{a}{2}(\hat{i} - \hat{j} + \hat{k})$$

$$\vec{A}_8 = \frac{a}{2}(\hat{i} + \hat{j} - \hat{k})$$

The primitive unit cell of lattice is a rhombohedron, formed by vectors  $\vec{A}_6, \vec{A}_7, \vec{A}_8$ . Hence volume of primitive unit cell in bcc lattice is

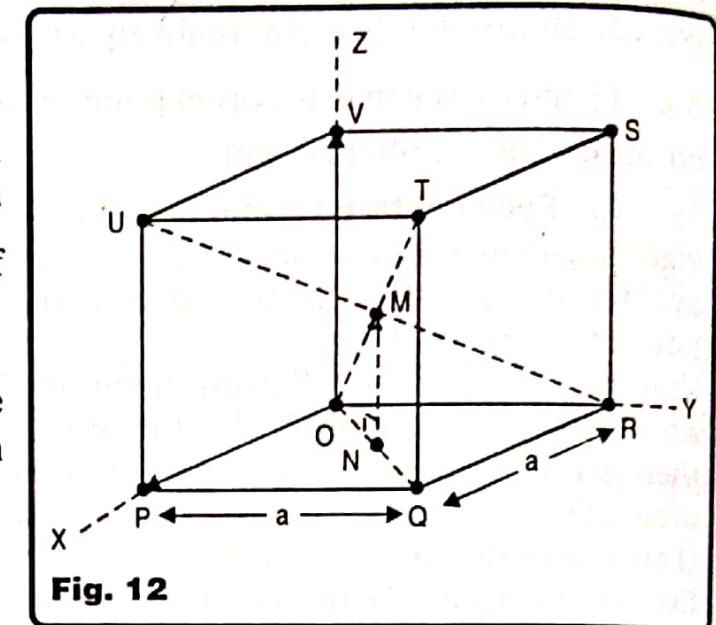


Fig. 12

$$\begin{aligned}
 V &= \vec{A}_6 \cdot (\vec{A}_7 \times \vec{A}_8) \\
 &= \frac{a^3}{8} \begin{vmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix} = \left(\frac{a^3}{8}\right) (4) \\
 &= \frac{a^3}{2}
 \end{aligned} \quad \dots(12)$$

(iii) **Face centered cubic.** A non primitive unit cell of fcc lattice is shown in fig. (13). The point M is nearest neighbour of corner point O. Let  $\vec{A}_1 = \vec{OM}$ . We consider X, Y, Z axes as shown in fig. (13). If 'a' is lattice constant then we have

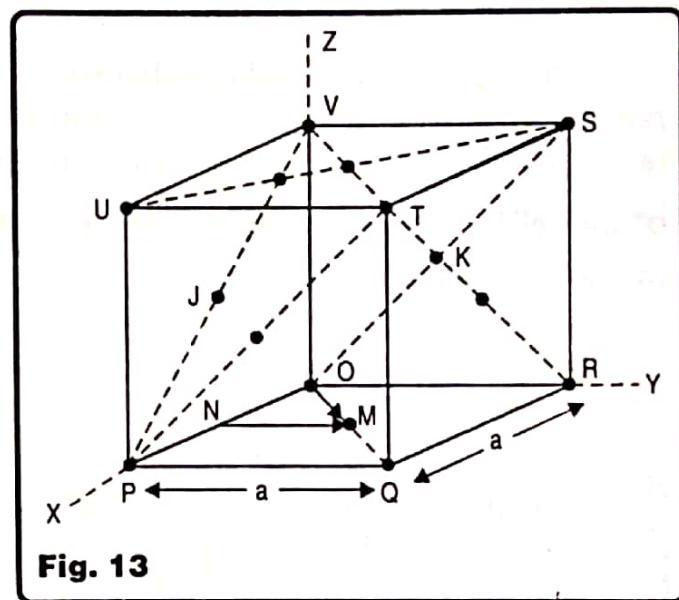
$$\vec{ON} = \frac{\vec{OP}}{2} = \frac{a}{2} \hat{i} \quad \dots(13)$$

and  $\vec{NM} = \frac{\vec{OR}}{2} = \frac{a}{2} \hat{j}$

$$\therefore \vec{OM} = \vec{ON} + \vec{NM} = \frac{a}{2} \left( \hat{i} + \hat{j} \right)$$

Similarly  $\vec{OJ} = \frac{a}{2} \left( \hat{i} + \hat{k} \right)$

and  $\vec{OK} = \frac{a}{2} \left( \hat{j} + \hat{k} \right)$



**Fig. 13**

The vectors  $\vec{OM}$ ,  $\vec{OJ}$ ,  $\vec{OK}$  form a primitive unit cell for fcc lattice. It is also a rhombohedron. Hence volume of primitive unit cell for fcc lattice is given as

$$\begin{aligned}
 V &= \vec{OM} \cdot (\vec{OJ} \times \vec{OK}) \\
 &= \left(\frac{a}{2}\right)^3 \begin{vmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{vmatrix} = \left(\frac{a^3}{8}\right)(2) = \frac{a^3}{4}
 \end{aligned} \quad \dots(14)$$

## (10) PACKING FACTOR

It is defined as, "the fraction of the volume of unit cell, that can be filled by atoms/molecules." It tells how tightly atoms are packed in a crystal. Higher value of packing factor implies more close packing of atoms. It can be calculated by dividing total volume of atoms contained in unit cell with the volume of unit cell.

Let  $r$  = radius of atom.

$N$  = number of atoms per unit cell

$V$  = volume of unit cell

Then packing factor is given as

$$f = \frac{N \times \frac{4\pi}{3} r^3}{V} \quad \dots(15)$$

Here we have assumed atom has hard sphere. We shall now find value of packing for a few unit cells.

(i) **Simple Cubic.** In a simple cubic lattice there is a lattice point at every corner of unit cell. When atoms are placed at these lattice points then corner atoms will touch each other because one corner atom is neighbour to another corner atom. This is shown in fig. (14). Only the atoms at four corners of one face are shown to avoid complexity. From fig., it is clear that

$$2r = a$$

$$\text{or } r = \frac{a}{2} \quad \dots(16)$$

This equation gives relation between atomic radius  $r$  and lattice constant ' $a$ ' for simple cubic lattice. Further the contribution of atom at corner of unit cell is only  $\frac{1}{8}$ . Hence total number of atoms in one unit cell are

$$N = 8 \times \frac{1}{8} = 1 \quad \dots(17)$$

Also volume is unit cell (cube) is given by

$$V = a^3 \quad \dots(18)$$

Put all these values from (16) – (18) in (15), we get

$$f = \frac{1 \times \frac{4\pi}{3} \times \frac{a^3}{8}}{a^3} = \frac{\pi}{6} = 0.52 \quad \dots(19)$$

Thus space filled by atoms is only 52% of available space.

(ii) **Body centered cubic.** In bcc lattice there is a lattice point at each corner of unit cell and one lattice point at the centre of unit cell. Since to every corner point has central point as its nearest neighbour so when atoms are placed at lattice points then every atom at corner will touch the central atom. One such situation is shown in fig. (15). It is clear from figure that

$$4r = AB \quad \dots(20)$$

where  $r$  = atomic radius

$AB$  = length of body diagonal

If  $a$  = lattice constant then from figure, we can obtain.

$$\begin{aligned} PB^2 &= PQ^2 + QB^2 \\ &= a^2 + a^2 = 2a^2 \end{aligned} \quad \dots(21)$$

and

$$\begin{aligned} AB^2 &= AP^2 + PB^2 \\ &= a^2 + 2a^2 \text{ (using 21)} \\ &= 3a^2 \end{aligned}$$

$$\therefore AB = \sqrt{3}a$$

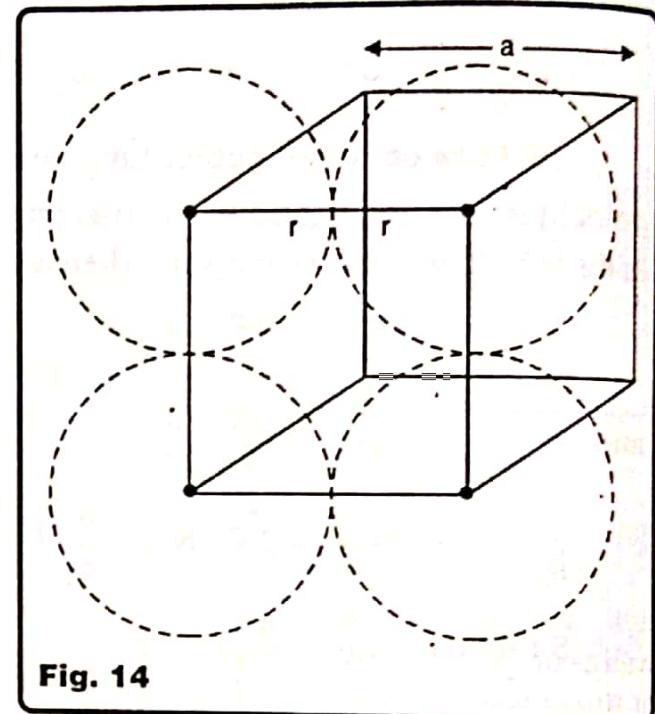


Fig. 14

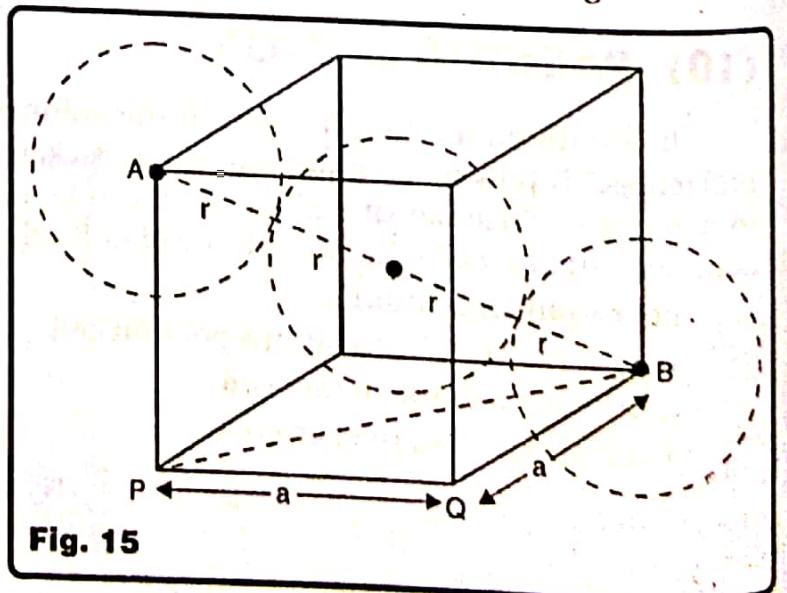


Fig. 15

Insert this value in (20), we get

$$\begin{aligned} 4r &= \sqrt{3} a \\ r &= \frac{\sqrt{3}}{4} a \end{aligned} \quad \dots(22)$$

$$\text{Number of atoms per unit cell } N = \left(8 \times \frac{1}{8}\right) + 1 = 2 \quad \dots(23)$$

$$\begin{aligned} V &= \text{volume of unit cell (cube)} \\ &= a^3 \end{aligned} \quad \dots(24)$$

Put values from (22) – (24) in equation (15), we get

$$\begin{aligned} f &= \frac{2 \times \frac{4\pi}{3} \left(\frac{\sqrt{3}}{4} a\right)^3}{a^3} \\ &= \frac{\sqrt{3}\pi}{8} \\ &= 0.68 \end{aligned} \quad \dots(25)$$

Hence space occupied by atoms is only 68% of available space.

(iii) **Face centered cubic.** In this lattice there is a lattice point at each corner of cube as well as at the centre of each face. Further nearest neighbour of a corner point is the lattice point at the centre of corresponding face. Hence when atoms are placed at lattice points then all corner atoms of one face will touch the atom placed at centre of that face. This situation is shown in fig. (16). From fig., it is clear that

$$4r = BC \quad \dots(26)$$

where  $r$  = atomic radius

and  $BC$  = length of diagonal of a face

If  $a$  = lattice constant, then we can write

$$\begin{aligned} BC^2 &= BA^2 + AC^2 \\ &= a^2 + a^2 = 2a^2 \\ \therefore BC &= \sqrt{2} a \end{aligned}$$

Insert this value in equation (26), we get

$$\begin{aligned} 4r &= \sqrt{2} a \\ r &= \frac{a}{2\sqrt{2}} \end{aligned} \quad \dots(27)$$

Also total number of atoms per unit cell are

$$N = 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4 \quad \dots(28)$$

The volume of cubic unit cell is

$$V = a^3 \quad \dots(29)$$

Put values from (27) – (29) in equation (15), we get

$$\begin{aligned} f &= \frac{4 \times \frac{4\pi}{3} \left(\frac{a}{2\sqrt{2}}\right)^3}{a^3} = \frac{\pi}{3\sqrt{2}} \\ &= 0.74 \end{aligned} \quad \dots(30)$$

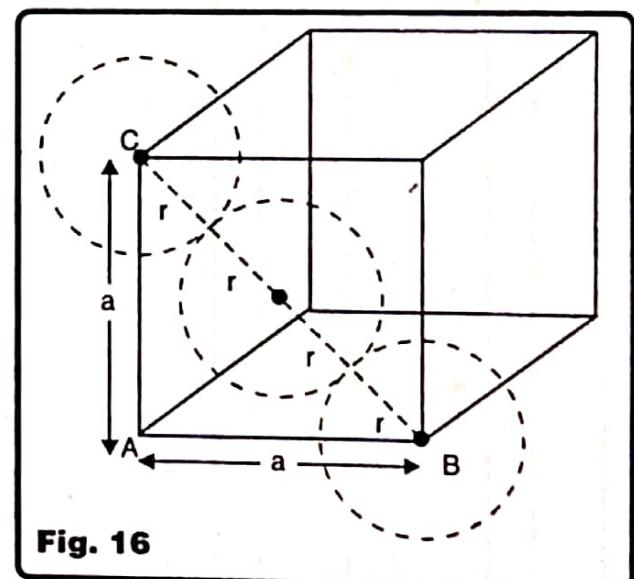


Fig. 16

Hence space occupied by atoms is only 74% of available space.

## (11) SOME SPECIAL CRYSTAL SYSTEMS

There are many crystal systems which have typical crystal structure. A few of them are discussed below :

(a) **Hexagonal closed Packed (HCP) structure.** Brief diagram of HCP unit cell is shown in fig. 17(a) and crystal structure with atoms/molecules would look like shown in figure 17(c). Here we have shown three layers of atoms one above the other. The central atom O' is surrounded by six atoms around it in its plane three atoms just below it and three above it (not shown in figure). Thus nearest neighbours are 12 or co-ordination number is 12. Further nearest neighbour separation is ' $a$ ' where ' $a$ ' is the length of each edge of hexagon.

Let  $C$  is the separation between two layers of hexagon shape. The number of atoms in each of hexagonal face is 7 (six at corners and one at the centre). Between each pair of hexagonal faces, there is a triangular shaped layer (like HIJ) containing three atoms. Positions of these atoms are at the line joining the centroids of the triangles formed by hexagonal faces as shown in fig. (17)(c).

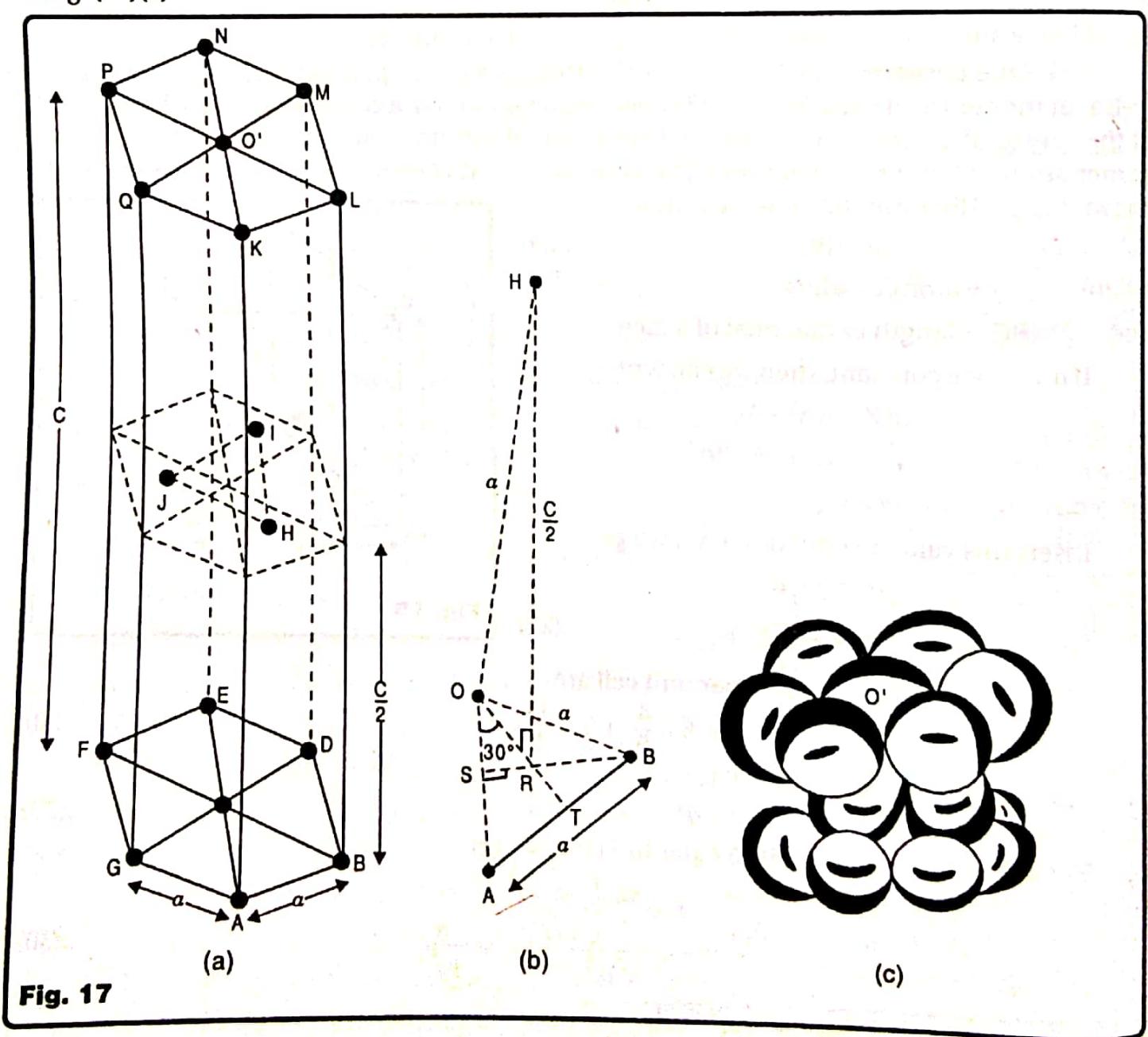


Fig. 17

Note that each atom like O, O', which is at the centre of hexagon is shared by two layers. So its contribution to unit cell is  $\frac{1}{2}$ . Further each atom at corner of hexagon is shared by six unit cells hence contribution of these atoms to unit cells is  $\frac{1}{6}$ . While each atom at points like H, I, J is totally confined to unit cell. Thus contribution of each such atom to unit cell is 1. Thus total number of atoms per unit cell are  $\frac{1}{2}(2) + \frac{1}{6}(6+6) + 1 \times (3) = 6$

Let us now calculate relation between length of edge ( $a$ ) and height ( $c$ ) of unit cell. From figure (17) (b), we have

$$OH = OA = OB = AB = a$$

$$RH = \frac{C}{2} \text{ (where R is centroid of triangle OAB)}$$

$$\angle AOT = 30^\circ$$

Now from figure, we have

$$\frac{OT}{OA} = \cos 30^\circ$$

$$\Rightarrow OT = OA \cos 30^\circ = \frac{\sqrt{3}a}{2} \quad \dots(31)$$

$$\text{Also } OR = \frac{2}{3}(OT)$$

$$= \frac{2}{3} \left( \frac{\sqrt{3}a}{2} \right) = \frac{a}{\sqrt{3}} \quad \dots(32)$$

By applying pythagoras theorems to  $\Delta HOR$ ,

$$\text{we get } (OH)^2 = (OR)^2 + (RH)^2$$

$$\Rightarrow a^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

$$\Rightarrow \frac{2}{3}a^2 = \frac{c^2}{4}$$

$$\therefore \frac{c}{a} = \sqrt{\frac{8}{3}} \quad \dots(33)$$

Now volume of unit cell is given by

$$V = (\text{area of base}) \times (\text{height})$$

$$= (\text{area ABDEFG}) \times (\text{BL})$$

$$= 6 \times (\text{area AOB}) \times (\text{BL})$$

$$= 6 \times \left( \frac{1}{2} \times AB \times OT \right) \times (\text{BL})$$

$$= 6 \times \frac{1}{2} \times a \times \frac{\sqrt{3}}{2} a \times c$$

$$= \frac{3\sqrt{3}}{2} a^2 \times c \quad \dots(34)$$

Since atoms A, B are in contact, if  $r$  is radius of each atom, then we have

$$\begin{aligned} 2r &= AB \\ \Rightarrow 2r &= a \\ \Rightarrow r &= \frac{a}{2} \end{aligned} \quad \dots(35)$$

$\therefore$  Volume of atoms contained in unit cell is

$$\begin{aligned} v &= 6 \times \frac{4\pi}{3} r^3 \\ &= 6 \times \frac{4\pi}{3} \times \frac{a^3}{8} = \pi a^3 \end{aligned} \quad \dots(36)$$

Thus packing factor of HCP structure (unit cell) is

$$\begin{aligned} f &= \frac{v}{V} = \frac{\pi a^3}{\frac{3\sqrt{3}}{2} a^2 c} \\ &= \frac{2\pi}{3\sqrt{3}} \frac{a}{c} = \frac{2\pi}{3\sqrt{3}} \times \sqrt{\frac{3}{8}} \\ &= \frac{2\pi}{3\sqrt{3}} \times \frac{\sqrt{3}}{2\sqrt{2}} = \frac{\pi}{3\sqrt{2}} = 0.74 \end{aligned}$$

Thus 74% of volume of unit cell is occupied in HCP. Hence HCP and FCC have equal and maximum value of packing factor. Some examples of HCP system are Mg, Zn and Cd.

(b) **Diamond structure.** The space lattice of diamond is FCC and primitive basic of crystal is a system of two identical carbon atoms placed at

$(0, 0, 0)$  and  $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$ . The unit cell is obtained by taking two interpenetrating FCC sublattices such that one sublattice has its origin at the point  $(0, 0, 0)$  and the origin of other is at  $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$ .

The co-ordination number is four. We know that number of atoms for each FCC unit cell is 4. Since there are two interpenetrating FCC cubes in unit cell of diamond, thus number of atoms per unit cell is  $4 + 4 = 8$ . Referring to figure 0 (18)(a), we get  $(AC)^2 = (AB)^2 + BC^2$

$$\begin{aligned} &= \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 \quad (\text{where } a = \text{edge of cube}) \\ &= \frac{a^2}{8} \end{aligned}$$

and

$$\begin{aligned} AD^2 &= AC^2 + CD^2 \\ &= \frac{a^2}{8} + \left(\frac{a}{4}\right)^2 = \frac{3a^2}{16} \end{aligned} \quad \dots(37)$$

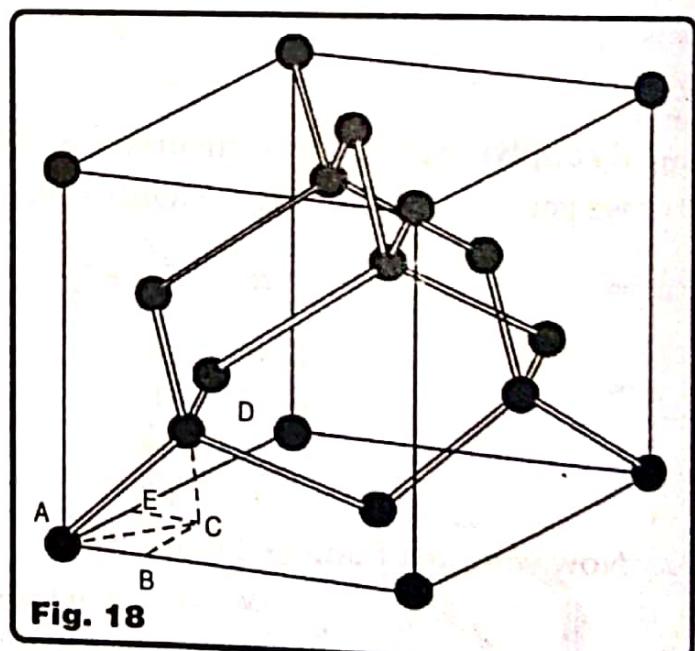


Fig. 18

Let  $r$  = atomic radius

$$\begin{aligned} \therefore AD &= 2r \\ \Rightarrow AD^2 &= 4r^2 \\ \Rightarrow \frac{3a^2}{16} &= 4r^2 \\ \Rightarrow r &= \frac{\sqrt{3}a}{8} \end{aligned} \quad \dots(38)$$

Thus packing further is given as

$$\begin{aligned} f &= \frac{8 \times \frac{4\pi}{3}r^3}{a^3} \quad (\text{The unit cell is cube}) \\ &= \frac{8 \times \frac{4\pi}{3} \times \frac{3\sqrt{3}a^3}{(8)^3}}{a^3} \\ \Rightarrow f &= \frac{\pi\sqrt{3}}{16} = 0.34 \end{aligned}$$

Thus 34% of space is occupied in diamond.

#### (c) Zinc Blende or Zinc Sulphide Structure.

We know that diamond structure may be considered as two FCC structures displaced from each other by one quarter of a body diagonal. All atoms are identical in case of diamond. The structure of ZnS reacts from diamond structure when Zn atoms are placed on one FCC lattice and S atoms on other lattice as shown in figure (19). The conventional cell is a cube. The coordinates of Zn atoms are  $(0, 0, 0)$ ,  $\left(0, \frac{1}{2}, \frac{1}{2}\right)$ ,  $\left(\frac{1}{2}, 0, \frac{1}{2}\right)$ ,  $\left(\frac{1}{2}, \frac{1}{2}, 0\right)$  and co-ordinates of S atoms are  $\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)$ ,  $\left(\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right)$ ,  $\left(\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right)$ ,  $\left(\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right)$ .

The number of atoms per unit cell is 8.

However one Zn atom and one S atom make one ZnS molecule. Thus there are 4 molecules of ZnS per unit cell. About each atom, there are four equidistant atoms of opposite kind arranged at the corners of a regular tetrahedron.

(d) Sodium Chloride Structure. The Bravais Lattice of sodium chloride is face centered cubic with one  $\text{Na}^+$  and one  $\text{Cl}^-$  ion separated by one half of the body diagonal of unit cube. One unit cell contains four molecules of  $\text{NaCl}$ . Each  $\text{Na}^+$  has six  $\text{Cl}^-$  ions as its nearest neighbours. Hence co-ordination number

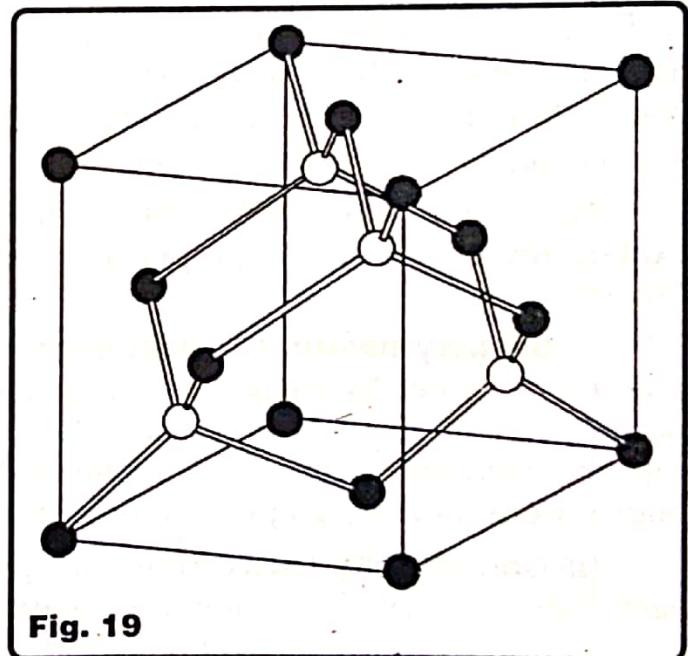


Fig. 19

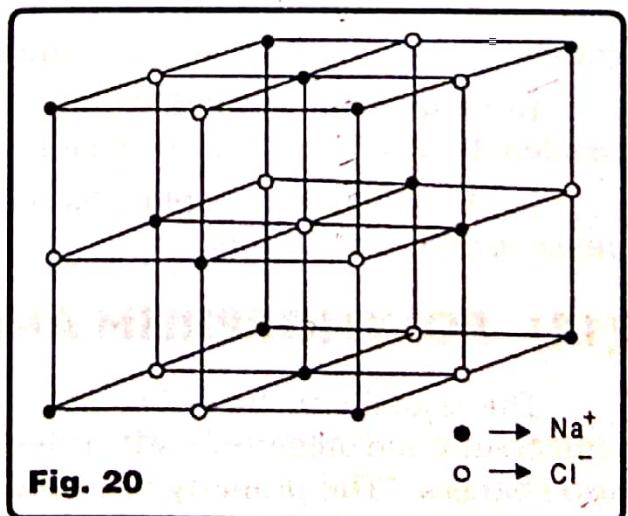


Fig. 20

is 6. The cube edge has value  $5.63\text{ \AA}$ . The structure of NaCl crystal is shown in fig. (20). The co-ordinates of  $\text{Na}^+$  and  $\text{Cl}^-$  ions in a cubic unit cell (with one corner considered as origin) are given below :-

$$\text{Cl}^- (0, 0, 0); \left(\frac{1}{2}, \frac{1}{2}, 0\right); \left(\frac{1}{2}, 0, \frac{1}{2}\right); \left(0, \frac{1}{2}, \frac{1}{2}\right)$$

$$\text{Na}^+ \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right); \left(0, 0, \frac{1}{2}\right); \left(0, \frac{1}{2}, 0\right); \left(\frac{1}{2}, 0, 0\right)$$

We may construct NaCl crystal structure by arranging  $\text{Na}^+$  and  $\text{Cl}^-$  ions alternatively at the lattice point of a simple cubic lattice also.

(e) **Graphite Structure.** Graphite, unlike diamond, has a two dimensional sheet like structure. Each carbon atom in graphite is  $sp^2$  hybridized. Each carbon atom is bonded to three other carbon atoms through covalent bonds forming hexagonal planar rings. The C—C covalent bond distance in rings is  $1.42\text{ \AA}$  indicating strong bonding. Thus, graphite has two dimensional sheet like polymeric rings. Each sheet or layer may be regarded as fused system of benzene rings. Any two successive sheets are about  $3.4\text{ \AA}$  apart. This large distance between the two successive layers does not permit the formation of covalent bonds. Different layers are held together by weak van der Waal's forces.

The structure discussed above can be used to explain the characteristic properties of graphite as follows :

(i) **Slippery nature.** Different layers in graphite are held together by weak van der Waal's forces. It permits sliding of one layer over another. This allows also the cleavage of the structure along the lines of planes. Consequently, graphite is soft and slippery and can be used as a lubricant.

(ii) **Conductivity.** Each carbon in graphite is  $sp^2$  hybridized. Thus one valence electron of each carbon atom is free to move from one point to other. The unhybridized orbitals containing one electron each overlap laterally to form  $p$ -bonds between adjacent layers. These electrons are delocalised and are quite free to move under the influence of heat and electric field. Thus, graphite is good conductor of heat and electricity.

(iii) **High melting point.** Within each layer, the carbon atoms are firmly bonded by strong covalent bonds. Therefore, the melting point of graphite is high (about  $3500^\circ\text{C}$ ).

(iv) **Low density.** Graphite has lower density than diamond due to the large distances between successive layers.

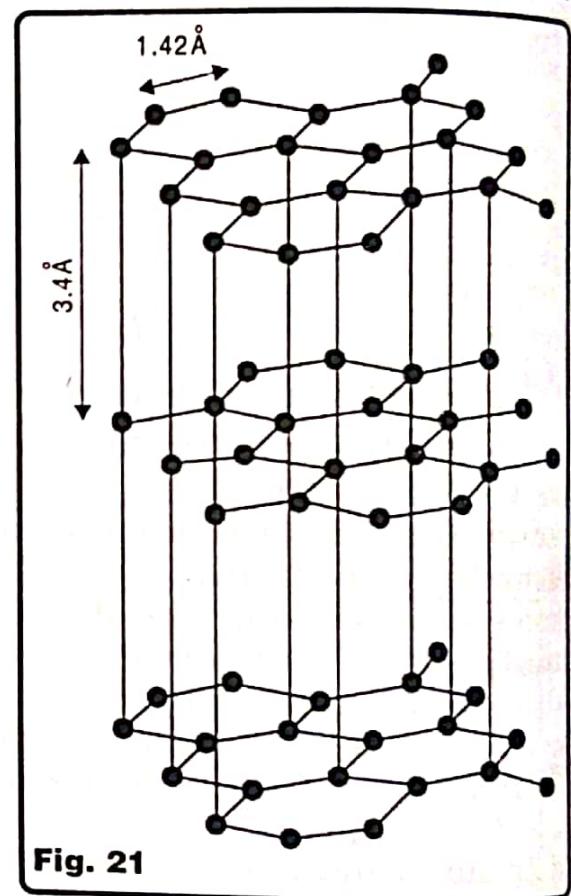


Fig. 21

## (12) POLYMORPHISM AND ALLOTROPY

The crystal structure of some solids is a function of external physical conditions like temperature and pressure i.e. when these physical conditions are changed, then crystal structure also changes. "The property of a solid to change from one crystal structure to another on

changing temperature and pressure is called polymorphism." In certain crystals these changes are reversible i.e. when original conditions of temperature and pressure are restarted than the crystal structure is also changed back to original structure at these conditions. This means during this process no chemical change takes place in the solid material. Only physical properties are changed. For example diamond and graphite are allotropic forms of carbon. Their crystal structures have been discussed in previous sections. The structure of diamond is a combination of two interpenetrating FCC lattices and all bonds are covalent bonds due to which diamond is bad conductor of electricity. On the other hand the carbon atoms in graphite form parallel layers. Each layers consist of hexagon shaped rings and bond length (length of each side of hexagon) is 1.42 Å. Two consecutive layers are separated by a distance of 3.4 Å. From fig. (31) we see that one carbon atom is connected to 3 other carbon atoms in same layer by covalent bonds. Since carbon has 4 bonding electrons out of which only 3 are used in covalent bonding, the fourth bonding electron is delocalized between three carbon bonds. Due to such electrons are free electrons and due to this graphite is good conductor of electricity.

Other examples of allotropic forms are cobalt (HCP at room temperature and FCC for temperature more than 477°C), iron, Zirconium, titanium etc.

### (13) CRYSTAL DIRECTIONS

For crystal structure Analysis, certain directions within the lattice are extremely important compared to other. Hence it becomes necessary to devise a method, which can specify all orientations uniquely. One such method was given by Miller. Various steps involved in this method are explained as follows :

(i) Consider any lattice point P and draw a vector from lattice point O, considered as origin to point P.

(ii) Draw three (and only three) non coplanar vectors parallel to fundamental translation vectors  $\vec{a}, \vec{b}, \vec{c}$  so that  $\vec{OP}$  can be completely described in terms of these. Let vector drawn parallel to OA, OB, OC axes are denoted as  $\vec{OM}, \vec{MN}, \vec{NP}$  respectively.

Then by polygon law of vectors we can write

$$\vec{OP} = \vec{OM} + \vec{MN} + \vec{NP} \dots (40)$$

$$\text{Let } \vec{OM} = m\vec{a},$$

$$\vec{MN} = n\vec{b}$$

$$\text{and } \vec{NP} = l\vec{c}$$

where  $m, n, l$  are positive or negative integers. Then equation (40) reduces to

$$\vec{OP} = m\vec{a} + n\vec{b} + l\vec{c}$$

(ii) Collect coefficients of  $\vec{a}, \vec{b}, \vec{c}$  and divide each of them by their HCF so as to reduce them to smallest integers  $u, v, w$

$$\text{i.e. } \frac{m}{\text{HCF}} = u, \frac{n}{\text{HCF}} = v, \frac{l}{\text{HCF}} = w$$

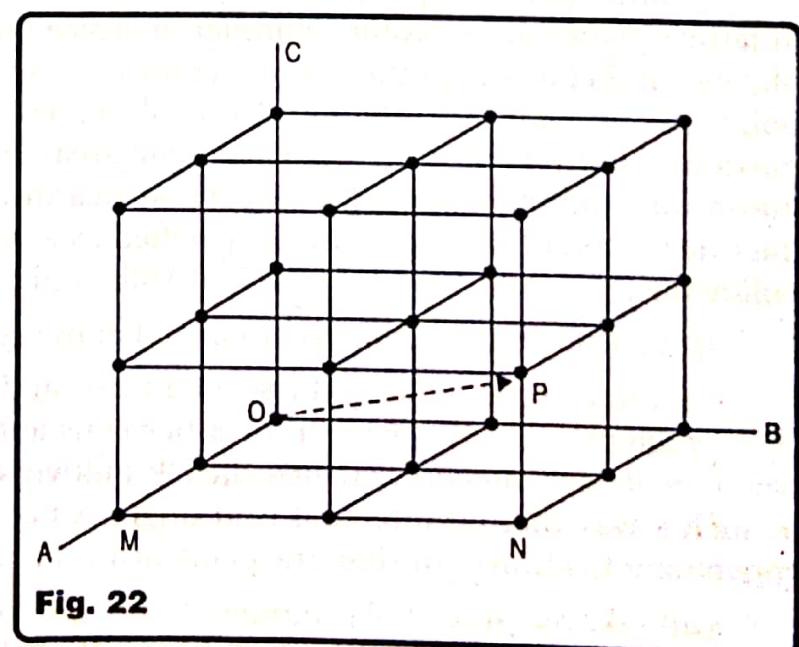


Fig. 22

(iv) The smallest integers  $u, v, w$  written in a square bracket as  $[uvw]$  represent the direction of  $\vec{OP}$ .

For example in fig. (17) we have

$$\begin{aligned}\vec{OP} &= \vec{OM} + \vec{MN} + \vec{NP} \\ &= 2\vec{a} + 2\vec{b} + 1\vec{c}\end{aligned}$$

$\therefore$  direction  $\vec{OP}$  is  $[221]$  (Note, 2, 2, 1 are already having no factor common so they directly represent direction of  $\vec{OP}$  & there is no need to divide by HCF here).

It should be noted that direction  $[442]$ ,  $[663]$  etc. are parallel to  $[221]$  and hence are same to each other.

(v) If one or more digits in square bracket are negative then that digit is represented by a bar over it.

For example direction  $[-101]$  is represented as  $[\bar{1}01]$ .

It should be noted that all possible directions having same set of integers are said to be equivalent and are written in angle brackets (carats) as  $\langle hkl \rangle$ . For example in fig. (22) the eight directs corresponding to  $OP, OQ, OR, OS, OJ, OK, OL$  and  $OM$  are  $[111], [\bar{1}11], [\bar{1}\bar{1}1], [1\bar{1}1], [\bar{1}\bar{1}\bar{1}], [1\bar{1}\bar{1}], [11\bar{1}]$  and  $[\bar{1}\bar{1}\bar{1}]$ . All these eight directions are equivalent w.r.t. origin and belong to a single family represented  $\langle 111 \rangle$ . Similarly the family  $\langle 110 \rangle$  consists of twelve equivalent directions. It is an exercise to the reader to express all these twelve directions.

## (14) MILLER INDICES

"A lattice plane is a plane passing through lattice points". For a given lattice a large number of lattice planes are possible. Number of lattice points per unit area is same for all lattice planes parallel to each other. However for two non parallel lattice planes number of lattice points per unit area are different. A crystal can be cut most easily along the plane, which has maximum number of lattice points per unit area. Due to this reason, the lattice planes having maximum number of lattice points per unit area are called 'cleavage planes'. In crystal analysis the orientation of a lattice plane is specified by a set of three numbers called Miller Indices. Following procedure is adopted to find Miller indices of a plane.

(i) Take any lattice point as origin and draw crystallographic axes  $OA, OB, OC$ .

(ii) Choose one plane of the set of interest and note down intercepts made by the plane on crystallographic axes in terms of lattice constants  $a, b, c$ . Let intercepts are  $ma, nb$  and  $lc$ , where  $m, n, l$  are integers and are called 'Primitives of the plane'. The plane should be chosen in such a way that no intercept is at origin. Since all parallel planes are exactly alike, it is convenient to always consider the plane nearest to origin.

(iii) Take reciprocals of primitives  $m, n, l$  and convert the fractions obtained into smallest set of integers by multiplying each of them with their LCM. These integers are denoted as  $h, k, l$  and enclosed by round brackets i.e.  $(hkl)$ . These integers are Miller indices of the plane.

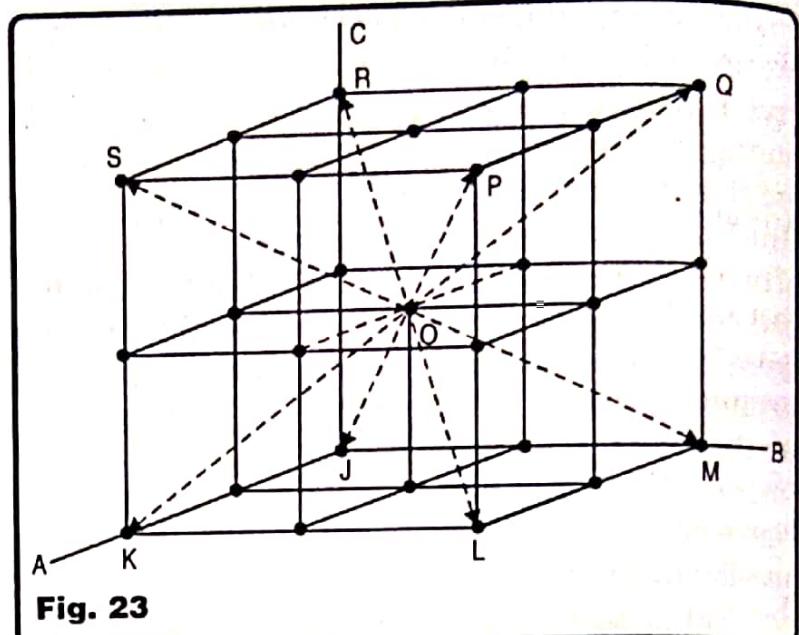


Fig. 23

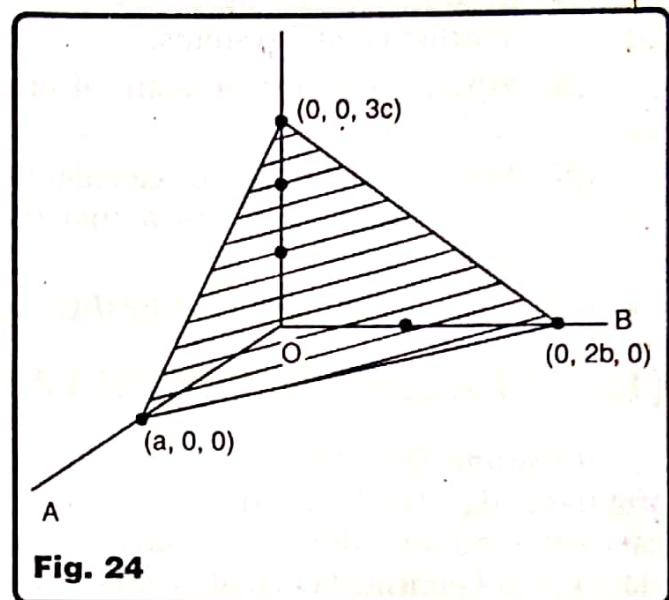
Note that if a plane cuts one or more crystallographic axis on the negative side of origin, then corresponding Miller index obtained is negative and is indicated by bar over the integer i.e.  $-h$  is represented as  $\bar{h}$  etc.

If a plane is parallel to one of crystallographic axis, then its intercepts will be  $\infty$  on that axis and hence corresponding Miller Index will be zero.

From above discussion, we may conclude that Miller Indices are the smallest integers, which have the same ratios with one another as the reciprocals of the intercepts expressed in terms of respective lattice constants. By taking reciprocals of intercepts, we bring all planes inside a single unit cell. This allows us to discuss all crystal planes in terms of planes passing through a single unit cell. Fig. (24) shows a lattice plane.

Its intercepts on OA, OB, OC axes are  $a$ ,  $2b$ ,  $3c$ . Primitives are 1, 2, 3. The reciprocals of primitives

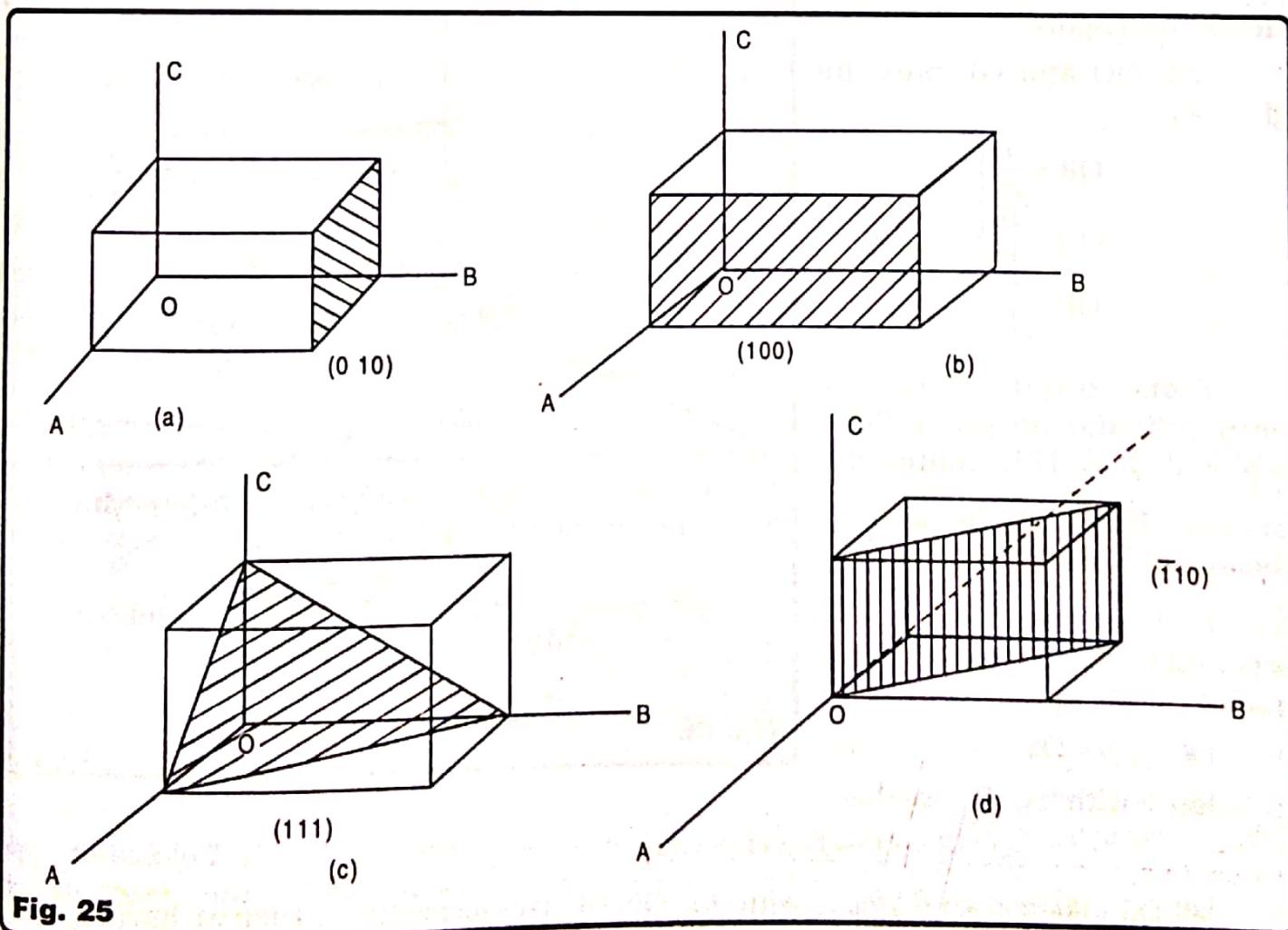
are  $1, \frac{1}{2}, \frac{1}{3}$ .



**Fig. 24**

Hence Miller indices of this plane are 6, 3, 2  $\equiv$  (632)

A few planes along with Miller Indices are shown in figure (25)



**Fig. 25**

It should be noted that family of planes having same integers  $h, k, l$  are denoted as  $\{hkl\}$ . Thus family of planes  $(2 \ 3 \ 3) \ (3 \ 2 \ 3) \ (3 \ 3 \ 2) \ (\bar{2} \ 3 \ 3) \ (3 \ \bar{2} \ 3) \ (3 \ 3 \ \bar{2}) \ (2 \ \bar{3} \ 3) \ (\bar{3} \ 2 \ 3) \ (3 \ 2 \ \bar{3}) \ (\bar{3} \ 3 \ 2) \ (3 \ \bar{3} \ 2)$  etc. is denoted by  $\{2 \ 3 \ 3\}$ .

Some important features of Miller Indices are as follows :

- In cubic crystals, the direction  $[hkl]$  is perpendicular to plane  $(hkl)$ . But this is not true in other crystal systems.
- When Miller integers are of double digits, these are separated by commas e.g.  $(7, 13, 15)$ .
- Miller indices are not calculated for a plane passing through origin. However its Miller indices are same as that of another plane parallel to it but not passing through origin.
- Various planes in a family  $\{hkl\}$  may or may not be parallel to each other.

## (15) SPACING BETWEEN LATTICE PLANES

Consider OA, OB, OC as crystallographic axes. Consider a plane JKL passing through origin (see fig. (21) (b) and another adjacent plane PQR parallel to it. Both planes being parallel, have same miller indices  $(hkl)$  (say). Let perpendicular distance between these two adjacent planes is ' $d$ '. Let plane PQR makes intercepts on crystallographic axes at points P, Q, R respectively (For more clear picture the intercept R is shown along negative side of OA axis. But this is not necessary).

Let  $a, b, c$  are lattice constants.  
Hence the lengths

OR, OQ and OP must be given as

$$\left. \begin{aligned} OR &= \frac{a}{h} \\ OQ &= \frac{b}{k} \\ OP &= \frac{c}{l} \end{aligned} \right\} \quad \dots(41)$$

From origin drop  $\vec{OS}$  perpendicular on plane PQR. Since PQR & JKL planes are parallel. Hence  $\vec{OS}$  is perpendicular to plane JKL also. Further length of  $\vec{OS}$  must be equal to separation ( $d$ ) between adjacent planes

$$i.e. \quad d = OS \quad \dots(42)$$

Join S with P, Q, R so that

$$\angle OSP = \angle OSQ = \angle OSR = 90^\circ \quad \dots(43)$$

Let  $\vec{OS}$  makes angle  $\theta_A, \theta_B, \theta_C$  with OA', OB, OC axes respectively. Then we have :-

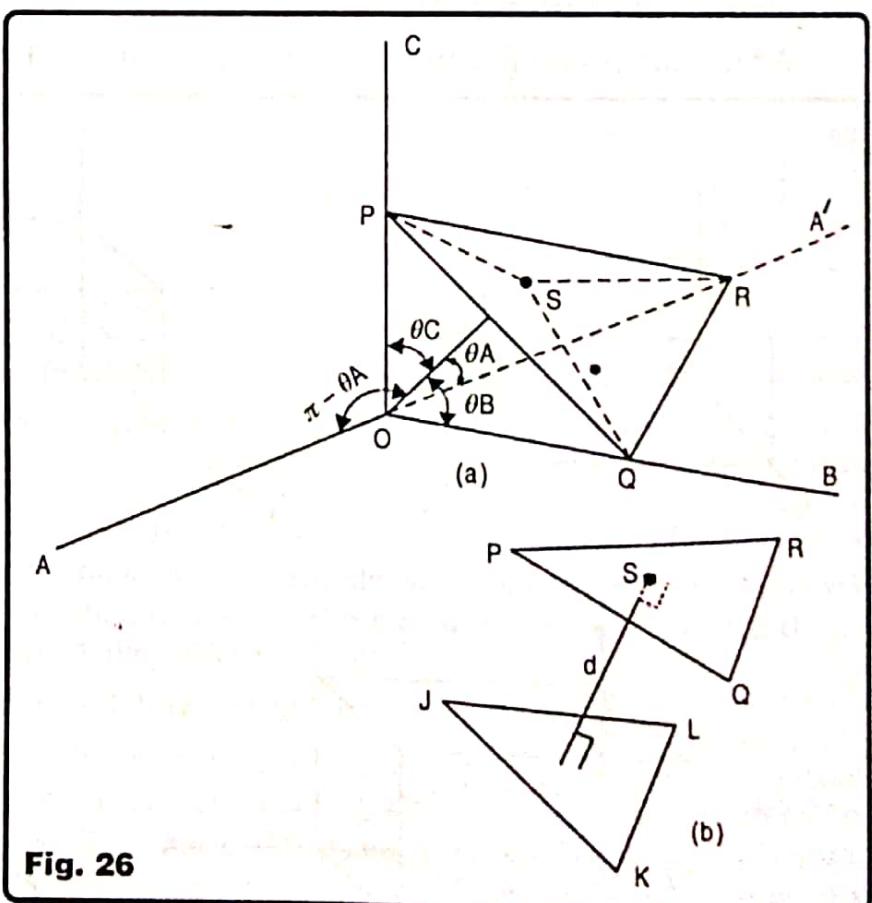


Fig. 26

In right angled triangle OSR

$$\begin{aligned}\cos \theta_A &= \frac{OS}{OR} \\ &= \frac{d}{a} \\ &= \frac{h}{\sqrt{a^2 + b^2}} \\ &= \frac{dh}{a} \quad \dots(44) \text{ using (41) and (42)}\end{aligned}$$

Similarly

$$\cos \theta_B = \frac{dk}{b} \quad \dots(45)$$

and

$$\cos \theta_C = \frac{dl}{c} \quad \dots(46)$$

Since  $\cos(\pi - \theta_A), \cos \theta_B, \cos \theta_C$  are direction cosines of  $\vec{OS}$ , hence we have the following standard result.

$$\begin{aligned}\cos^2(\pi - \theta_A) + \cos^2 \theta_B + \cos^2 \theta_C &= 1 \\ \Rightarrow \cos^2 \theta_A + \cos^2 \theta_B + \cos^2 \theta_C &= 1 \\ \Rightarrow d^2 \left( \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right) &= 1 \quad (\text{using (44) - (46)}) \\ \Rightarrow d &= \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}} \quad \dots(47)\end{aligned}$$

Equation (47) gives separation between lattice planes.

(i) For tetragonal system  $a = b$

$$\therefore (47) \Rightarrow d = \frac{1}{\sqrt{\frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}}}$$

(ii) For cubic system  $a = b = c$

$$\therefore (47) \Rightarrow d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

**Example 1.** X-rays of wavelength  $0.71 \text{ \AA}$  are reflected from the  $(110)$  plane of a rock salt crystal ( $a = 2.82 \text{ \AA}$ ). Calculate the glancing angle corresponding to second order reflection.

**Solution.**

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{2.82 \text{ \AA}}{\sqrt{1^2 + 1^2 + 0}} = 2.0 \text{ \AA}$$

By Bragg's Law

$$\sin \theta = \frac{n\lambda}{2d} = \frac{2 \times 0.71 \text{ \AA}}{2 \times 2.0 \text{ \AA}}$$

$$\Rightarrow \theta = 20^\circ 42'$$

**Example 2.** Find the atomic spacing in a crystal of rock salt ( $\text{NaCl}$ ) for which unit cell is simple cubic and there is one  $\text{NaCl}$  molecule for unit cell. The density of rock salt is

$2.16 \times 10^3 \text{ kg m}^{-3}$  and average masses of Na and Cl atoms are respectively  $3.82 \times 10^{-26} \text{ kg}$  and  $5.89 \times 10^{-26} \text{ kg}$ .

**Solution.** Let  $M$  = molecular weight of crystal

$$\rho = \text{density of crystal}$$

$$\text{Volume per mole of crystal} = \frac{M}{\rho}$$

There are  $2N$  ions in 1 mole ( $\because$  each unit cell contains one  $\text{Na}^+$  and one  $\text{Cl}^-$  ion). Here  $N = 6.023 \times 10^{23}$ .

$$\text{Thus volume associated with each ion} = V' = \frac{V}{2N} = \frac{M}{2\rho N} \quad \dots(i)$$

Let  $d$  = distance between two ions = plane spacing

$$\therefore \text{Volume of elementary cube of NaCl} = d^3 \quad \dots(ii)$$

Comparing (i) & (ii) we get

$$d^3 = \frac{M}{2\rho N}$$

$$\Rightarrow d = \left( \frac{M}{2\rho N} \right)^{1/3}$$

$$\text{For NaCl crystal} \quad \frac{M}{N} = \frac{M_{\text{Na}}}{N} + \frac{M_{\text{Cl}}}{N}$$

$$= 3.82 \times 10^{-26} + 5.89 \times 10^{-26} = 9.71 \times 10^{-26} \text{ kg}$$

$$\rho = 3.16 \times 10^3 \text{ kg/m}^3$$

$$\text{Thus} \quad d = \left( \frac{9.71 \times 10^{-26}}{2 \times 2.16 \times 10^3} \right)^{1/3} = 2.82 \text{ \AA}$$

**Example 3.** Show that for a cubic crystal direction  $[hkl]$  is normal to plane  $(hkl)$ .

**Solution.** A cubic system is an orthogonal system. Hence we can take crystallographic axes as X, Y, Z axes. We consider OA direction as X-axis, OB as Y axis and OC as Z-axis as shown in fig. (27). Hence fundamental translation vectors are given as

$$\begin{cases} \vec{a} = a\hat{i} \\ \vec{b} = b\hat{j} \\ \vec{c} = c\hat{k} \end{cases} \quad \dots(i)$$

$$\text{Where } c = b = a \quad \dots(ii)$$

(For cubic system)

Let  $[hkl]$  is the direction specified by  $\overrightarrow{OR}$ . Then  $\overrightarrow{OS}$  is given as  $\overrightarrow{OS} = h\vec{a} + k\vec{b} + l\vec{c}$

$$= h\hat{i} + k\hat{j} + l\hat{k} \quad \dots(iii)$$

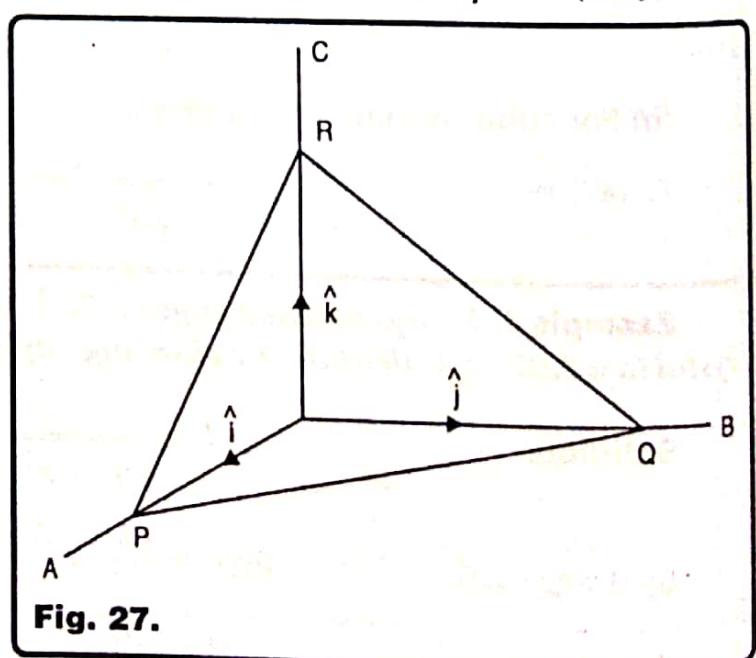


Fig. 27.

Now consider a plane whose Miller indices are  $(hkl)$ . This means it makes intercepts  $\frac{a}{h}, \frac{b}{k}, \frac{c}{l}$  on OA, OB, OC axes.

Hence

$$\vec{OP} = \frac{a}{h} \hat{i} \quad \dots(iv)$$

$$\vec{OQ} = \frac{b}{k} \hat{j}$$

$$\vec{OR} = \frac{c}{l} \hat{k}$$

Any vector within the plane is  $\vec{PQ}$  and by  $\Delta$  law of vectors, we have  $\vec{PQ} = \vec{OQ} - \vec{OP}$

$$= \frac{b}{k} \hat{j} - \frac{a}{h} \hat{i}$$

Now

$$\begin{aligned} \vec{OS} \cdot \vec{PQ} &= \left( ha \hat{i} + kb \hat{j} + lc \hat{k} \right) \cdot \left( \frac{b}{k} \hat{j} - \frac{a}{h} \hat{i} \right) \\ &= -a^2 + b^2 \\ &= -a^2 + a^2 \\ &= 0 \end{aligned} \quad (\because b = a \text{ for cubic system})$$

This means  $\vec{OS}$  is perpendicular to  $\vec{PQ}$ . But  $\vec{OS}$  is direction  $[hkl]$  and  $\vec{PQ}$  lies in plane  $(hkl)$ . Hence direction  $[hkl]$  is normal to plane  $(hkl)$  for a cubic crystal.

**Example 4.** Obtain the Miller indices of a plane having intercepts  $2a, -3b, 5c$ .

**Solution.** Primitives =  $2, -3, 5$

$$\text{Reciprocals} = \frac{1}{2}, -\frac{1}{3}, \frac{1}{5}$$

$$\text{Smallest integers} = 15, -10, 6$$

$\therefore$  Miller indices are  $(15, \overline{10}, 6)$

**Example 5.** A plane makes intercepts of  $1\text{\AA}$ ,  $2\text{\AA}$ , and  $3\text{\AA}$ . On the crystallographic axes of an orthorhombic crystal with  $a : b : c = 3 : 2 : 1$ . Determine the Miller Indices of the plane.

**Solution.** Let primitives are  $m, n, l$

$$\left. \begin{array}{l} ma = 1\text{\AA} \\ nb = 2\text{\AA} \\ lc = 3\text{\AA} \end{array} \right\} \quad \dots(i)$$

And

$$a : b : c = 3 : 2 : 1$$

$$\therefore a = 3k, b = 2k, c = k \text{ (where } k \text{ is some constant)}$$

$$\left. \begin{array}{l} m(3k) = 1 \\ n(2k) = 2 \\ l(k) = 3 \end{array} \right\} \quad \dots(ii)$$

$$\Rightarrow \frac{1}{m} = 3k$$

$$\frac{1}{n} = k$$

$$\frac{1}{l} = \frac{k}{3}$$

Converting them to least integers (multiply each factor by  $\frac{3}{k}$ ), we get  $(hkl) = (931)$  Ans.

**Example 6.** Calculate interplanar distance between  $(1\ 1\ 1)$  and  $(0\ 1\ 2)$  planes. Given that crystal system is cubic having lattice constant  $a$ . Also compare the atomic density of planes.

**Solution.**

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

∴

$$d_{111} = \frac{a}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{a}{\sqrt{3}}$$

And

$$d_{012} = \frac{a}{\sqrt{0+1+4}} = \frac{a}{\sqrt{5}}$$

The atomic density (no. of atoms per unit area of lattice plane) is given by

$$\rho = \frac{nd}{V}$$

where

$n$  = number of atoms in unit cell

$d$  = interplanar separation

$V$  = Volume of unit cell

∴

$$\frac{\rho_{111}}{\rho_{012}} = \frac{d_{111}}{d_{012}} = \frac{\sqrt{2}}{3} \text{ Ans.}$$

**Example 7.** Atomic radius of copper is  $1.28 \text{ \AA}$ . Its crystal structure is fcc. Find density of copper if its atomic weight is 63.54.

**Solution.**

$$r = 1.28 \text{ \AA}$$

For fcc lattice

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

∴

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

$$a^3 = (2\sqrt{2} r)^3$$

$$= 16\sqrt{2} r^3$$

$$= 47.43 \times 10^{-30} \text{ m}^3$$

For fcc structure  $N$  = no. of lattice points per unit cell = 4

$$M = \text{Atomic weight} = 63.54 \text{ g} = 63.54 \times 10^{-3} \text{ kg}$$

$$N_A = 6.023 \times 10^{23}$$

∴

$$\rho = \frac{MN}{a^3 N_A}$$

$$= \frac{63.54 \times 10^{-3} \times 4}{6.023 \times 10^{23} \times 47.43 \times 10^{-30}}$$

$$= 8.897 \times 10^3 \text{ kg m}^{-3}$$

**Exercise 1.** Determine Miller Indices of a plane, that makes intercepts  $3\text{\AA}$ ,  $2\text{\AA}$ ,  $4\text{\AA}$  on coordinate axes of an orthorhombic crystal with  $a : b : c = 4 : 2 : 3$  [Ans. (16, 6, 9)]

**Exercise 2.** For a fcc lattice, molecular weight is 62, density is  $6200 \text{ kg m}^{-3}$ . Calculate lattice constant  $a$ . [Ans.  $4.05 \text{ \AA}$ ]

**Exercise 3.** Calculate atomic density (number of atoms per unit area of lattice plane) in (111) plane of a bcc crystal having lattice constant  $a$ .

$$\left[ \text{Ans. } \frac{1}{a^2 \sqrt{3}} \right]$$

**Exercise 4.** The molecular weight of NaCl is 58.46 and density is  $2167 \text{ kg m}^{-3}$ . Calculate its lattice constant. Given structure of NaCl crystal is fcc with four NaCl molecules in unit cell. [Ans.  $5.64 \text{ \AA}$ ]

## **SHORT ANSWER TYPE QUESTIONS**

**Q. 1. What do you mean by crystallography?**

**Ans.** It is the branch of Physics, which deals with study of geometrical form and physical properties of crystalline solids.

**Q. 2. What do you mean by X-ray crystallography?**

**Ans.** It is the branch of Physics, which deals with study of crystal structure, texture, behaviour and the identification of crystals by method involving use of X-rays. It is also called Crystal Analysis.

**Q. 3. Amorphous solids do not possess sharp melting points. Why?**

**Ans.** The bonds in amorphous solids vary in strength because of lack of long range order. When an amorphous solid is heated, the weakest bond break at lower temperature than the other. Thus different bonds break up at different temperatures. Hence amorphous solids do not possess sharp melting points.

**Q. 4. Why steel bars and sheets formed by cold rolling are much harder than formed by hot rolling?**

**Ans.** Strongly heating (annealing) a solid decrease dislocations (defects) in the crystal and try to bring out more ordered arrangement of atoms. Due to this material becomes more ductile and it is easy to deform it. Hence steel bars or sheets formed by cold rolling cannot be easily deformed and are much harder than formed by hot rolling.

**Q. 5. What is the limitation of Laue's method ?**

**Ans.** It cannot be used to find lattice spacing. It can only tell the symmetry properties of crystal.

**Q. 6. What do you mean by reciprocal lattice?**

**Ans.** We know that slope of a plane is determined by its normal. In a collection of large number of planes, which may be parallel or non parallel, we can represent them by their normals.

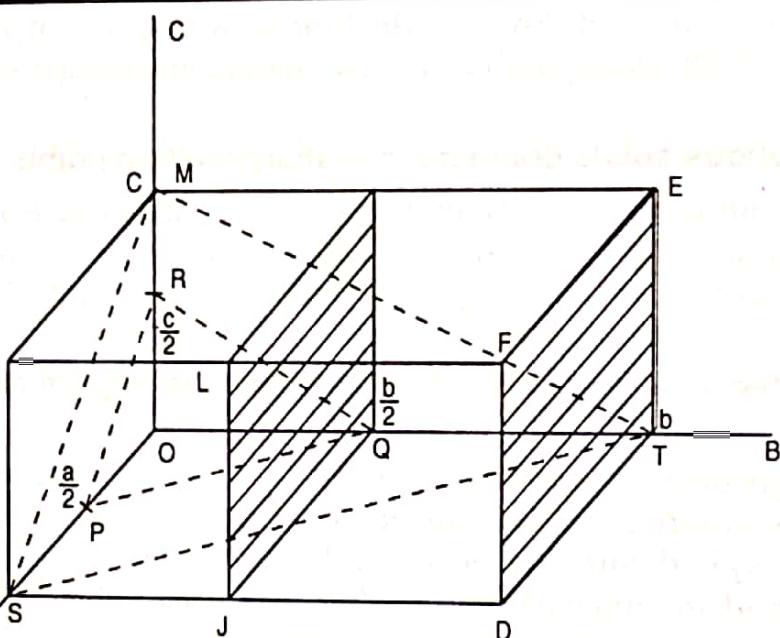
"If the length assigned to each normal is proportional to reciprocal of interplanar spacing of the plane, then the points marked at the end of their normal drawn from a common origin is called Reciprocal lattice."

Following procedure is adopted to construct a reciprocal lattice.

- (i) Take a lattice point in direct lattice as origin.
- (ii) Draw one normal for one family of parallel planes in such a way that it must pass through origin. If there are  $N$  families of parallel planes, then there will be  $N$ -normals passing through origin.

- (iii) Find interplanar spacing for one family of parallel planes and take its reciprocal  $\frac{1}{d_{hkl}}$ . Using a compass draw arcs (starting from origin) on the normal at distance  $2\pi \times \frac{1}{d_{hkl}}$ .
- (iv) Mark the points of intersection of arc with normal.
- (v) Draw such points for all the N-normals. In this way the arrangement of points obtained in space is a reciprocal lattice.

For example in fig. (28), we have shown two sets of parallel planes in the direct lattice. One set of parallel planes is recognised as (010), (020), (030) etc., while second set as (111), (222) etc. In fig. (29), the reciprocal lattice is shown corresponding to these two sets of planes. Since planes (010) etc. are normal to OB axis so the normal passing through origin for these planes is OB' axis itself. Lattice points on this normal are separated by  $\frac{2\pi}{d_{010}}$  distance. Similarly

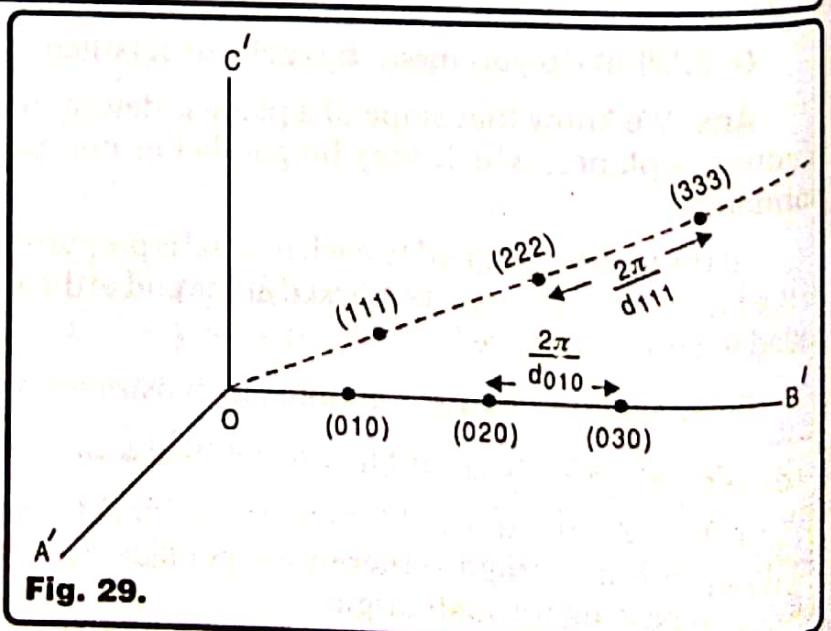


**Fig. 29**

for the planes (111) etc., normal passing through origin is shown by dotted line and two consecutive points on this line are separated by  $\frac{2\pi}{d_{111}}$ .

**Q. 9. What are reciprocal Lattice Vectors? Show that reciprocal lattice of a simple cubic system is itself a simple cubic lattice.**

**Ans.** (i) "A vector, whose magnitude is equal to  $2\pi$  times the reciprocal of interplanar spacing (i.e.  $\frac{2\pi}{d_{hkl}}$ ) and direction is parallel to



**Fig. 29.**

the normal drawn on  $(hkl)$  plane is called Reciprocal Lattice Vector." These are denoted by  $\vec{A}, \vec{B}, \vec{C}$  and these are related to fundamental translation vectors of direct lattice as :-

$$\vec{A} = 2\pi \left( \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right) \quad \dots(i)$$

$$\vec{B} = 2\pi \left( \frac{\vec{c} \times \vec{a}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right) \quad \dots(ii)$$

$$\vec{C} = 2\pi \left( \frac{\vec{a} \times \vec{b}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \right) \quad \dots(iii)$$

The dimensions of reciprocal lattice vectors  $\vec{A}, \vec{B}, \vec{C}$  are of  $(\text{length})^{-1}$ .

(ii) For a simple cubic lattice, we have

$$\begin{aligned} \vec{a} &= a\hat{i} \\ \vec{b} &= a\hat{j} \\ \vec{c} &= a\hat{k} \quad (\because b=c=a) \\ \therefore (1) \Rightarrow \vec{A} &= 2\pi \left( \frac{a\hat{j} \times a\hat{k}}{a\hat{i} \cdot (a\hat{j} \times a\hat{k})} \right) \\ &= \frac{2\pi}{a} \hat{i} \end{aligned}$$

Similarly

$$\vec{B} = \frac{2\pi}{a} \hat{j}$$

$$\vec{C} = \frac{2\pi}{a} \hat{k}$$

Clearly  $|\vec{A}| = |\vec{B}| = |\vec{C}| = \frac{2\pi}{a}$

Also  $\vec{A}, \vec{B}, \vec{C}$  are mutually perpendicular. Hence we find that reciprocal lattice to a simple cubic lattice is itself a simple cubic lattice with lattice constant  $\frac{2\pi}{a}$ .

## QUESTIONS

1. What do you mean by space lattice and unit cell of crystal ?
2. What is co-ordination number ? Calculate the co-ordination number for simple cubic and body centered cubic lattices.
3. Explain the term 'Miller Indices'. What is their role in crystal structure ? Give the important features of Miller Indices.

4. What do you mean by packing factor ? Calculate packing factor for body centered cubic, simple cubic and face centered cubic.
5. Discuss the terms (a) Co-ordination number (b) Space Lattice.
6. Describe any seven systems of crystals with suitable diagrams and give the relation of lengths of axis and the relation of angles between the axes of a unit cell in each type.
7. Write a brief note on space lattice.
8. Define and explain atoms per unit cell.
9. Briefly discuss space lattice and reciprocal lattice.
10. Write a brief note on packing factor.
11. Define crystal lattice, Basis and Crystal Structure.
12. What do you understand by Miller Indices. Hence find interplanar spacing between  $(hkl)$  planes.
13. Show that reciprocal lattice of Simple Cubic System is itself simple cubic.
14. Define monocrystal and polycrystal.
15. What do you mean by Cohesive Energy.
16. What are various kinds of bonds in crystalline solids ?
17. What do you mean by Crystal Translation Vector ?
18. Mention rules to construct Wigner Seitz cell.
19. Define Bravais Lattice.
20. What is importance of symmetry properties in crystal structure analysis ?
21. Obtain a relation between lattice constant and density in case of cubic lattice.
22. Define atomic density of a lattice plane and write an expression for it.
23. Find out volume of primitive unit cell for cubic system.
24. What do you mean by crystal directions ? How a direction is specified?
25. Discuss crystal structure of diamond.
26. Discuss crystal structure of HCP and find packing.
27. What do you mean by crystal defects ? Give its types and discuss these briefly.

