Crystal Structure

Matter consists by one or more elements or their chemical compounds, exists in nature in the form of solid, liquid and gaseous states. Among these solids have definite size and shape of corresponding volume. The Solid State physics is the branch of physics dealing with physical properties of solids, particularly crystals, including the behaviour of electrons in these solids. The solids may be broadly classified as crystalline and non-crystalline depending upon the arrangement of atoms or molecules.

The crystalline state of solids is characterized by regular or periodic arrangement of atoms or molecules. Most of the solids are crystalline in nature. The crystalline state is low energy state and crystalline solids may be subdivided into single crystals and poly crystalline solids. In single crystals, the periodicity of atoms extends throughout the material as the case of diamond quartz, mica, etc. A polycrystalline material is an aggregate of a number of small crystallites with random orientations separated by well defined boundaries. The small crystallites are known as grains and boundaries as grain boundaries. Periodicity of individual crystallites is interrupted at grain boundaries, yet the polycrystalline form of material may be more stable compared with the single crystal form. Most of the metals and ceramics exhibit polycrystalline structure.

The noncrystalline or amorphous solids are characterized by the completely random arrangement of atoms or molecules. The periodicity extends upto a distance of a few atomic distances only. These solids are short range order. Glass, rubbers & plastics are amorphous materials.

The science which deals with the study of geometrical forms and physical properties of crystalline solids is called crystallography. The study of crystallography is necessary to understand the strong correlation between the structure of a material and its physical properties.

Crystal lattice and translation vectors:-

Before describing the arrangement of atoms in a crystal, it is always convenient to describe the arrangement of imaginary points in space which has a definite relationship with the atoms of the crystal. This set of imaginary points forms a framework on which the actual crystal structure is based. Such an arrangement of infinite number of imaginary points in three dimensional space with each point having identical surroundings is known as space lattice.

The term identical surroundings means that the lattice has the same appearence when viewed from a point $\vec{r}$ in the lattice as it has when viewed from any other point $\vec{r}'$ w.r.to some arbitrary origin. This is possible only if the lattice contains a small group of points, called pattern unit, which repeats itself in all directions by means of a translation operation $\vec{T}$ given by

$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \quad \ldots \quad (1)$$

where n_1, n_2, n_3 are arbitrary integers and the vectors $\vec{a}$, $\vec{b}$, and $\vec{c}$ are called the fundamental translation vectors. Thus we have

$$\vec{r}' = \vec{r} + \vec{T} = \vec{r} + n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \quad \ldots \quad (2)$$

In case of perfect lattice eqn(2) holds good and in imperfect lattice this eqn(2) not obey welly. The translation vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$ are also called the crystal axes or basis vectors.

For simple understanding a part of a two-dimensional lattice as shown in fig. (1). The translation vectors $\vec{a}$ and $\vec{b}$ can be chosen in a number of ways. Two such possibilities are shown in this figure, where two sets $\vec{a}_1, \vec{b}_1$ and $\vec{a}_2, \vec{b}_2$ of translation vectors are drawn. Considering first the translation vectors $\vec{a}_1$ and $\vec{b}_1$, the point $\vec{R}'$ can be obtained from $\vec{R}$ using the translation ~~vectors~~ operation given by

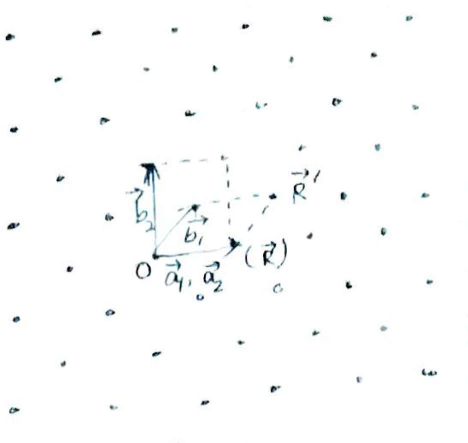


Fig (1)

$$\vec{T} = 0.\vec{a}_1 + 1.\vec{b}_1$$

which contains integral co-efficients. Thus $\vec{R}'$ is related to $\vec{R}$ by the equation

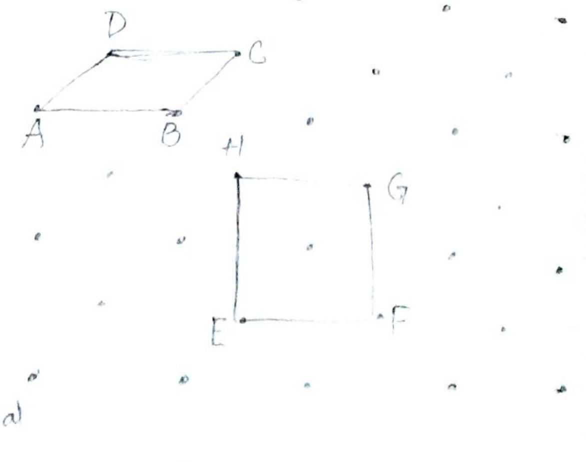
$$\vec{R}' = \vec{R} + \vec{T} = \vec{R} + 0.\vec{a}_1 + 1.\vec{b}_1$$

Such translation vectors which produce a translation operation containing integral co-efficients are called primitive translation vectors. Considering the set $\vec{a}_2, \vec{b}_2$ the point $\vec{R}'$ can be got from $\vec{R}$ by using the equation

$$\vec{R}' = \vec{R} + \frac{1}{2}\vec{a}_2 + \frac{1}{2}\vec{b}_2$$

which contain non-integral co-efficients of $\vec{a}_2$ and $\vec{b}_2$. Such translation vectors contain non-integral co-efficients are called non-primitive translation vectors. Non integral coefficients not in accordance with the periodicity of the crystal.

Unit cell :-



The parallelograms formed by translation vectors may be regarded as building blocks for constructing the complete lattice and are known as unit cells of the lattice. For a three dimensional lattice the unit cells are of the

Fig (2)

Thus a unit cell may be defined as the smallest unit of the lattice which, on ~~Compet~~ continuous repitition, generates the complete lattice. Both primitive and non-primitive translation vectors may be used to construct a unit cell. Accordingly, a unit cell is named as a primitive unit cell or non-primitive unit cell. In fig (2) the parallelogram ABCD represents a two-dimensional primitive cell, where as EFGH represents nonprimitive cell. Primitive unit cell is the smallest volume cell. All the primitive cells, the lattice points lying at its corners. So, the effective number of lattice points in a primitive cell is one. A non-primitive cell may have the lattice points at the corners as well as other positions. Therefore the effective number of lattice points in a non-primitive cell is more than one.

Wigner-Seitz Primitive cell :- A primitive cell can also be constructed using the following procedure.

(i) connect a given lattice point to all the near-by lattice points

(ii) Draw normals at the midpoints of the lines connecting the lattice as shown in fig.(3)

The smallest volume enclosed by the normal planes is the Wigner-Seitz primitive unit cell. The volume of this type primitive cell having $\vec{a}$, $\vec{b}$ and $\vec{c}$ as the fundamental translation vectors is :

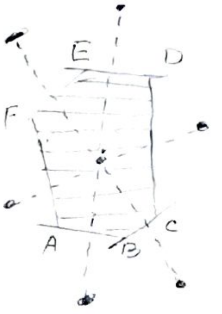


Fig.(3)

$$V = |\vec{a}\cdot\vec{b}\times\vec{c}|$$

Basis or Pattern:- ~~The~~ ~~sp~~ For a lattice to represent a crystal structrure, we associate every lattice point with one or more atoms in a regular fashion. Such an atom or a group of atoms is called the basis or pattern. When the basis is repeated with correct periodicity in all directions, it gives the actual crystal structure. The crystal structure is real, while the lattice is imaginary. Thus

$$\boxed{\text{lattice + basis = Crystal Structure}}$$

Fig (4)

Fig (4) shows the basis or pattern representing each lattice point. It is observed that from the figure that a basis consists of three different atoms. It can also be observed that the basis is identical in composition [illegible]. The number of

Symmetry operations:- A Symmetry operation is that which transforms the crystal to itself, i.e. a crystal remains invariant under such symmetry operation. These operations are translation, rotation, reflection and inversion. The translation operation applies to lattices only while all other remaining operations and their combinations apply to all objects and are collectively known as point symmetry operations.

(i) **Translations:-** The translation symmetry follows from the orderly arrangement of a lattice. It means that a lattice point $\vec{r}$, under lattice translation vector operation $\vec{T}$, gives another point $\vec{r}'$ which is exactly identical to $\vec{r}$ i.e.

$$\boxed{\vec{r}' = \vec{r} + \vec{T}}$$

(ii) **Rotation:-** A lattice is said to possess the rotation symmetry if its rotation by an angle θ about axis (or a point in two dimension) transforms the ~~body~~ lattice into itself. Also, since the lattice always remains invariant by a rotation of 2π, the angle 2π must be an integral multiple of θ, i.e.

$$n\theta = 2\pi$$

$$\text{or, } \theta = \frac{2\pi}{n}$$

The factor n takes integral value, and is known as multiplicity of rotation axis. A rotation corresponding to the value of n is called n-fold rotation. Fig.(5) shows that six fold rotation axis about the point O.

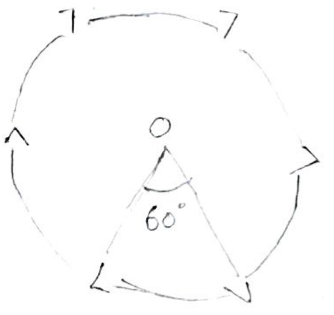


Fig (5.)

Absence of five fold Symmetry axis:-

Consider a lattice row XPQY in Fig.(6). Let the lattice translation be 'a' and the lattice have n-fold rotation axis symmetry. Let the vectors PX and QY rotate by an angle $\phi_n = \frac{360°}{n}$ in the clockwise and anticlockwise direction respectively. The tips of the vectors P_1 and Q_1 in new positions must be lattice points if the lattice were to possess n fold rotation axis of Symmetry. As per the definition, rotation operation must leave the lattice invariant. clearly, P_1Q_1 must be parallel to PQ and must be equal to an integral multiple of the lattice translation 'a'; i.e. $P_1Q_1 = ma$ where m is an integer.

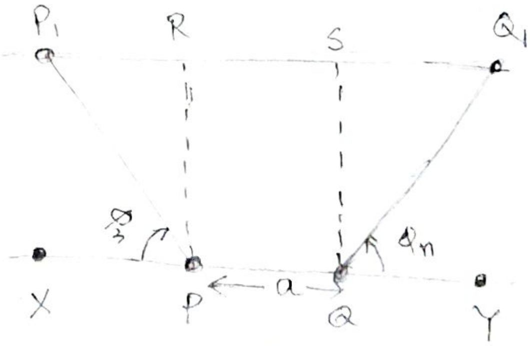


Fig. 6.

Thus $\cos\phi_n = \frac{P_1R}{PP_1}$

or. $P_1R = PP_1\cos\phi_n = a\cos\phi_n$

and $SQ_1 = a\cos\phi_n$.

Therefore, $P_1Q_1 = P_1R + SQ_1 + RS$

$= 2a\cos\phi_n + a = ma$

Thus, $1 + 2\cos\phi_n = m$

or. $\cos\phi_n = \frac{m-1}{2} = \frac{N}{2}$ N = is an integer.

N	$\frac{N}{2}$	$\cos\phi_n$	ϕ_n	$n = \frac{360^\circ}{n}$
-2	-1	-1	180°	2
-1	$-\frac{1}{2}$	$-\frac{1}{2}$	120°	3
0	0	0	90°	4
$+1$	$+\frac{1}{2}$	$+\frac{1}{2}$	60°	6
$+2$	$+1$	$+1$	360°	1

So, in this table $n = 5$ is absent. So it is proved that five fold rotational symmetry axis is impossible.

Point groups:- We have seen that there are mainly four types of symmetry, i.e. translation, rotation, reflection and inversion. The last three operations are point operations and their combinations give certain symmetry elements which collectively determine the symmetry of space around a point. The group of such symmetry operations at a point is called a point group. There are 10 and 32 different point groups in 2D and 3D - lattices respectively.

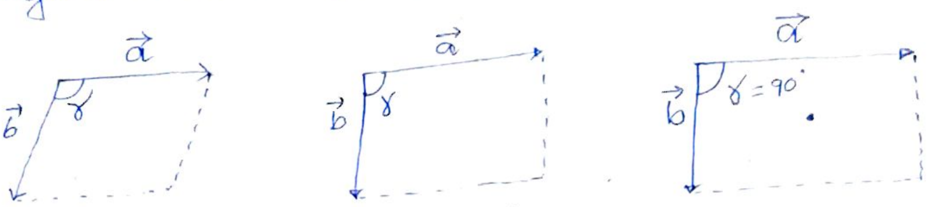
Space group:- In a crystal, point group symmetry operations can also be combined with translation symmetry elements, provided they are compatible. Such combinations are called space groups. There are 17 and 230 distinct space groups possible in two and three dimensions respectively.

Bravais lattice:- There are a number of ways in which an actual crystal may be built up and atoms piled together resulting many crystal structures. But each of the structures consists of some fundamental patterns repeated at each point of a space lattice. The scheme of repetitions of space lattice are very limited number; while the possible crystal structures are almost unlimited. But it was shown by Bravais in 1843 that there are only 14 different arrays of lattice. These are known as Bravais space lattice. In 2D, there are 5 different Bravais lattices.

Crystal system:- These Bravais lattices further become parts of 4 and 7 distinct crystal systems in 2D and 3D respectively.

(i) Two-Dimensional lattices:-

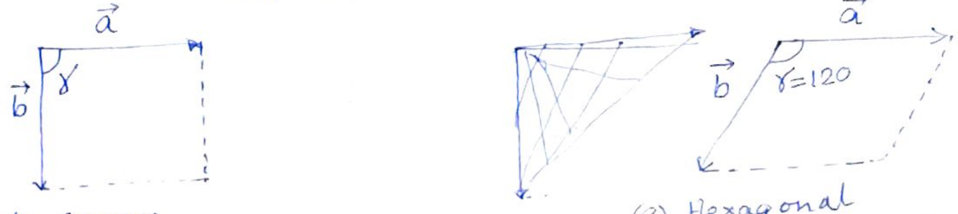
The four crystal systems of two-dimensional space are oblique, rectangular, square and hexagonal. The rectangular crystal system has two Bravais lattices, namely, rectangular primitive and rectangular centred. These lattices are shown in fig (7).



(a) oblique
$a \neq b$, $\gamma \neq 90°$

(b) Rectangular primitive
$a \neq b$, $\gamma = 90°$

(c) Rectangular centred
$a \neq b$, $\gamma = 90°$



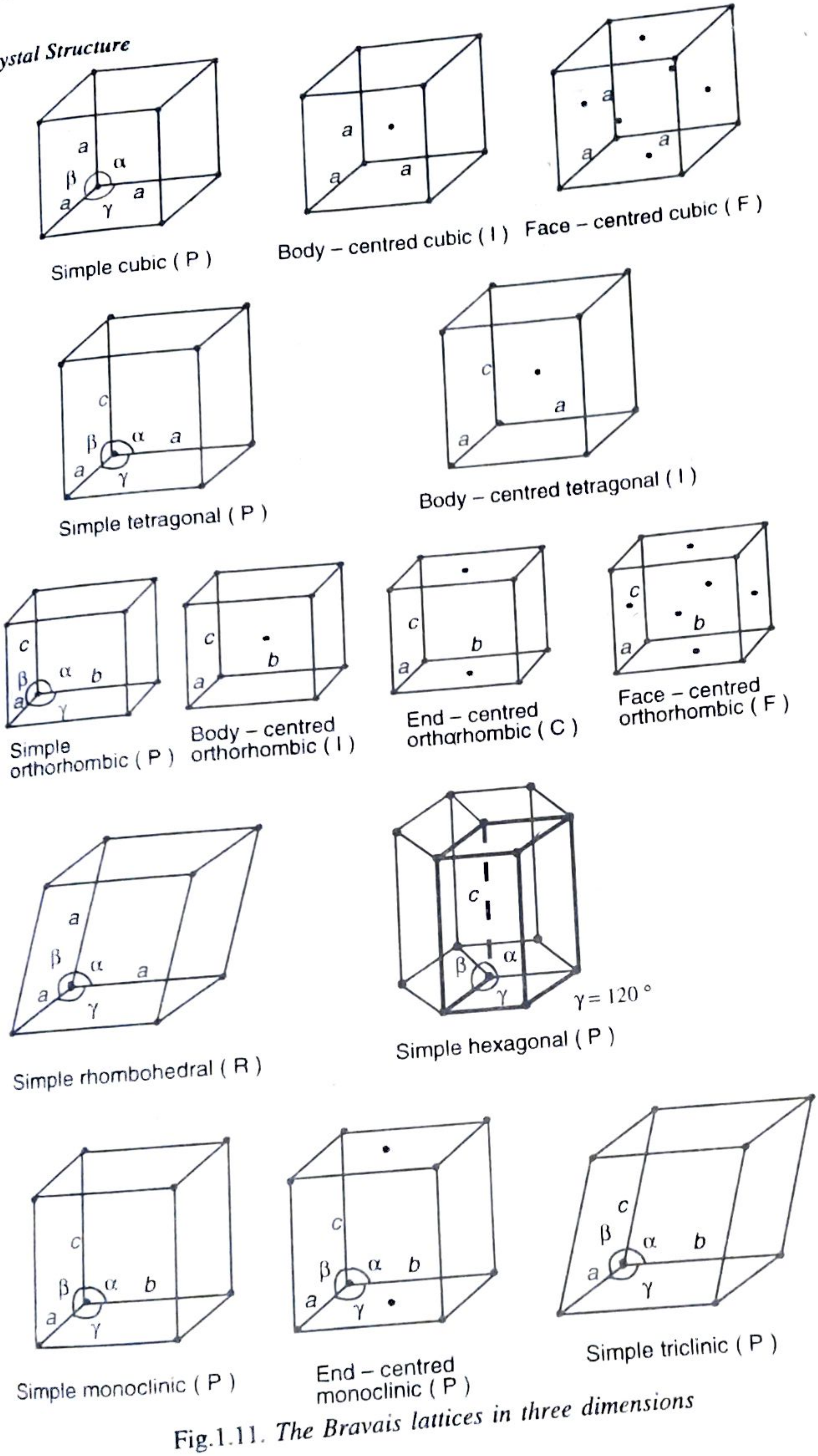
(d) square
$a = b$, $\gamma = 90°$

(e) Hexagonal
$\vec{a} = \vec{b}$, $\gamma = 120°$

Fig(7)

(ii) Three-Dimensional lattices:- All the seven crystal systems of three dimensional space and the corresponding Bravais lattices are listed in Table (1). in the decreasing order of symmetry. The crystallographic axes $\vec{a}$, $\vec{b}$ and $\vec{c}$ drawn from one of the lattice points determine the size and shape of a unit cell. The angles α, β and γ represent the angles between the vectors $\vec{b}$ and $\vec{c}$, $\vec{c}$ and $\vec{a}$, and $\vec{a}$ and $\vec{b}$ respectively. The lengths a, b and c and angles α, β and γ are collectively known as lattice parameter or lattice constants of a unit cell.

S.No.	Crystal System	Lattice parameter	Bravais lattice	Common abbreviation	Lattice Symbol	Examples
1.	Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90°$	Simple Body-centred Face-centred	sc bcc fcc	P I F	Polonium Cr, CsCl Cu, Ag, Pb
2.	Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	Simple Bodycentred	st bct	P I	β-Sn TiO_2
3	Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	Simple Body centred End-centred Face centred	so bco eco fco	P I C F	Ga Fe_3C
4	Trigonal	$a = b = c$ $\alpha = \beta = \gamma \neq 90°$	simple	–	P	As, Sb, Bi
5	Hexagonal	$a = b \neq c$ $\alpha = \beta = 90°$ $\gamma = 120°$	Simple	–	P	Mg, Zn, Cd
6	Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$	Simple End-centred	–	P C	$CaSO_4 \cdot 2H_2O$
7	Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90°$	Simple	–	P	$K_2Cr_2O_7$



Simple cubic (P)

Body – centred cubic (I)

Face – centred cubic (F)

Simple tetragonal (P)

Body – centred tetragonal (I)

Simple orthorhombic (P)

Body – centred orthorhombic (I)

End – centred ortharhombic (C)

Face – centred orthorhombic (F)

Simple rhombohedral (R)

Simple hexagonal (P)

Simple monoclinic (P)

End – centred monoclinic (P)

Simple triclinic (P)

Fig.1.11. *The Bravais lattices in three dimensions*

a, b and c

Lattice directions, Planes and Miller indices:-

In a crystal there exists directions and planes which contain a large number of atoms. It is necessary to locate these directions and planes for crystal analysis. In fig(9) two directions are shown by arrows in two-dimensions. These directions pass through the origin O and end A and B respectively. The directions are described by giving the coordinates of first whole numbered point (x, y) through which each of directions passed. For instance, OA has direction (1,1) and for OB (3,1). In 3D, the directions are described by the co-ordinates of the first whole numbered point (x, y, z). Generally, square brackets are used to indicate a direction. A few directions are shown below.

OA [110] , OB [010], OC [111] , OD [201] , OE [221]

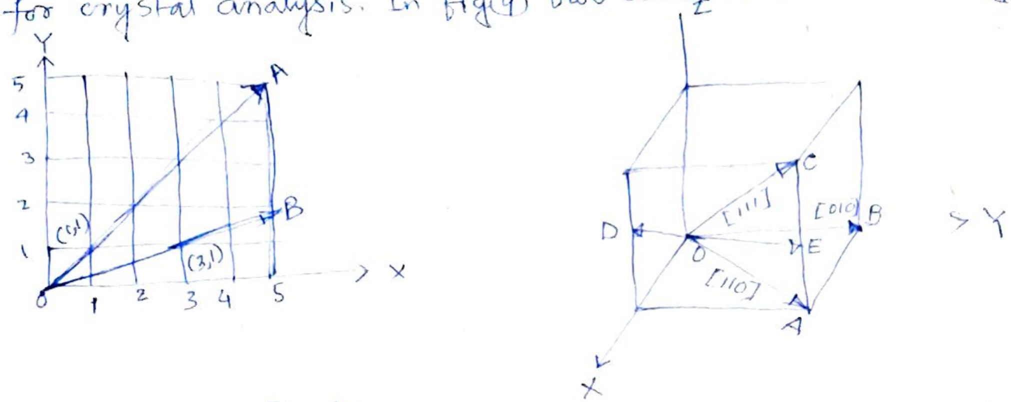


Fig.(9)

Lattice planes:- The crystal lattice may be regarded as made-up of an aggregate of a set of parallel equidistant planes, passing through the lattice points, which are known as lattice planes. For a given lattice, the lattice planes can be chosen in different ways as shown in fig(10).

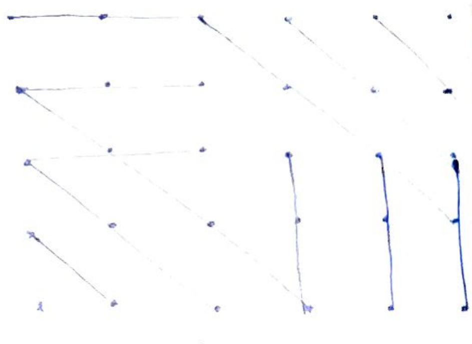


Fig.(10)

Miller Indices:- The scheme to represent the orientation of planes in a lattice was first introduced by Miller, a British crystallographer. The indices of planes are therefore known as the Miller indices. The Miller indices of a plane in general are written as (hkl)

The steps in the determination of Miller indices of a plane are as follows with the aid of fig.(11).

(i) Determine the co-ordinates of the intercepts made by the plane along the three crystallographic axes.

x	y	z
2a	3b	c

(ii) Express the intercepts as multiples of the unit cell dimensions, or lattice parameters along the axes i.e.

(iii) Determine the reciprocals of these numbers

$\frac{1}{2}$ $\frac{1}{3}$ $\frac{1}{1}$

(iv) Reduce these reciprocals to the smallest set of integers enclosed them in brackets

$6\times\frac{1}{2}$ $6\times\frac{1}{3}$ $6\times\frac{1}{1}$

(3 2 6)

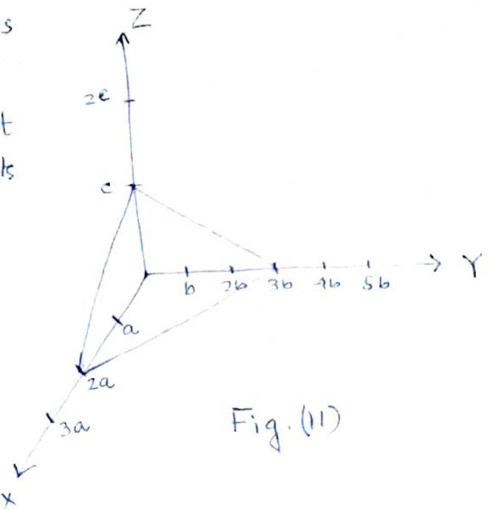


Fig. (11)

Thus, Miller indices may be defined as the reciprocals of the intercepts made by the plane on the crystallographic axes when reduced to smallest numbers.

Important features of Miller indices of crystal planes are

(i) All the parallel equidistant planes have the same Miller indices. Thus the Miller indices define a set of parallel planes.

(ii) A plane parallel to one of the co-ordinate axes has an intercept of infinity.

(iii) If the Miller indices of two planes have the same ratio (i.e. 844 and 422 or 211), then the planes are parallel to each other.

(iv) If (hkl) are the Miller indices of a plane, then the planes cuts the axes into equal h, k, l segments respectively.

(v) Miller indices of the plane is the perpendicular to the direction having the corresponding number same. As an example (010) are the Miller indices of the plane is the perpendicular to [010] directions.

Interplanar spacing:-

The spacing between parallel adjacent planes is d_{hkl}. The Miller indices of the plane is (hkl). The intercepts of the (hkl) plane on $\vec{a}$, $\vec{b}$ and $\vec{c}$ axes are $\frac{a}{h}$, $\frac{b}{k}$ and $\frac{c}{l}$ respectively shown in fig (12).

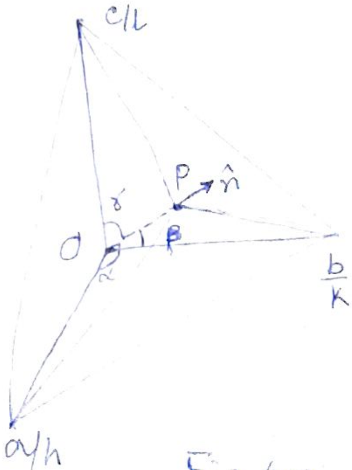


Fig. (12)

$$d_{hkl} = OP = \frac{a}{h}\cos\alpha = \frac{b}{k}\cos\beta = \frac{c}{l}\cos\gamma \quad \ldots (1)$$

α, β and γ are the angles between the normal to the plane and $\vec{a}$, $\vec{b}$ and $\vec{c}$ axes respectively.

If $\hat{n}$ be unit vector ~~to the~~ normal to the plane, then $a\cos\alpha$, $b\cos\beta$ and $c\cos\gamma$ may be written as

$\hat{n}.\vec{a}$, $\hat{n}.\vec{b}$ and $\hat{n}.\vec{c}$ respectively.

Therefore eqn (1) become

$$d_{hkl} = \frac{\hat{n}\cdot\vec{a}}{h} = \frac{\hat{n}\cdot\vec{b}}{c} = \hat{n}\cdot\vec{c} \quad \ldots (2)$$

In an orthogonal lattice, taking X, Y, Z axes along $\vec{a}$, $\vec{b}$ and $\vec{c}$ directions respectively, the equation of the plane (hkl) with intercepts $\frac{a}{h}$, $\frac{b}{k}$ and $\frac{c}{l}$ is

$$f(x,y,z) = \frac{hx}{a} + \frac{ky}{b} + \frac{lz}{c} = 1$$

For a surface $f(x,y,z) = \text{const}$, $\vec{\nabla} f$ represents the vector normal to

$$\hat{n} = \frac{\vec{\nabla} f}{|\vec{\nabla} f|} = \frac{\frac{h}{a}\hat{i} + \frac{k}{b}\hat{j} + \frac{l}{c}\hat{k}}{\left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right)^{1/2}}$$

From eqn (2), we have

$$d_{hkl} = \frac{\hat{n}\cdot\vec{a}}{h} = \frac{\left[\frac{h}{a}\hat{i} + \frac{k}{b}\hat{j} + \frac{l}{c}\hat{k}\right]\cdot\frac{a\hat{i}}{h}}{\left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right)^{1/2}}$$

$$\boxed{d_{hkl} = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}} \quad \cdots\cdots (3)$$

For a cubic crystal, $a = b = c$,

$$\boxed{d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}} \quad \cdots\cdots (4)$$

Metallic crystal Structures :- Three relatively simple crystal structures are found for the most common metals; body centred cubic, face centred cubic and hexagonal close packed.

Simple cubic Structure (SC)

In a simple cubic lattice, there is one lattice point at each of the eight corners of unit cell. If we consider one corner lattice point as centre, this atom is surrounded by six nearest neighbours and hence the co-ordination number of a simple cubic lattice is six. The corner atom is shared by eight unit-cells.

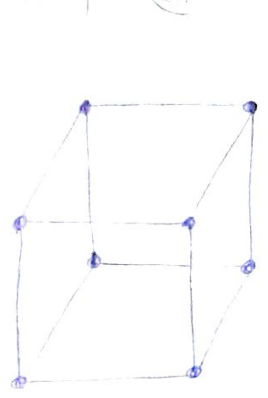
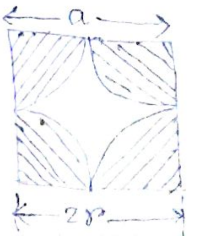


Fig. ⑬

Hence the share of each corner atom to a unit cell is one-eighth of an atom. So, the number of atoms in one unit cell is $\frac{1}{8}\times 8 = 1$. So the effective number of lattice point in a SC lattice is one. Thus SC is a primitive cell.

Hence the nearest neighbour distance, $2r = a$ (Fig. 14) where 'a' unit cell dimension and r is the radius of the atom.



Co-ordination number. $N = 6$

Nearest neighbour distance, $2r = a$

Lattice distance $a = 2r$

Number of atoms per unit cell $(n) = \frac{1}{8} \times 8 = 1$

Volume of the atom in a unit cell, $(v) = \frac{4}{3}\pi r^3$

Volume of the unit cell, $V = a^3 = (2r)^3$

Hence packing fraction, the fraction of the volume of a unit cell occupied by atoms is known as packing factor (PF).

Therefore in SC lattices,

$$PF = \frac{v}{V} = \frac{\frac{4}{3}\pi r^3}{a^3}$$

$$= \frac{4}{3} \times \frac{\pi r^3}{8 r^3}$$

$$= \frac{\pi}{6} = 0.52 = 52\%$$

SC is a loosely packed structure.

Body centered cubic Structure (bcc)

In this structure, in a unit cell, there are 8 atoms in eight corners and another atom at the body centre.

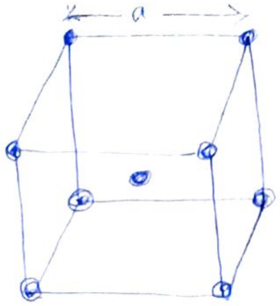
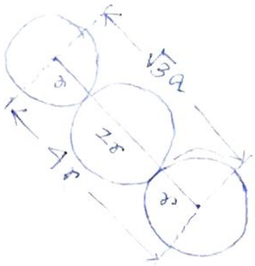


Fig. (15)



Number of atoms per unit cell in a bcc Structure is $\frac{1}{8} \times 8 + 1 = 2$. Each corner atoms touch the centre atom. So, Co-ordination number is 8.

According to fig.(15),

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

$$\therefore a = \frac{4r}{\sqrt{3}} \text{ and } (2r) = \frac{\sqrt{3}a}{2}$$

So, Co-ordination number = 8

Nearest neighbour distance, $2r = \frac{\sqrt{3}a}{2}$

Lattice Constant, $a = \frac{4r}{\sqrt{3}}$

No. of atoms per unit cell $= 8 \times \frac{1}{8} + 1$

$= 2$

Volume of atoms per unit cell, $v = 2 \times \frac{4}{3}\pi r^3$

Volume of unit cell, $V = a^3 = \frac{64 r^3}{3\sqrt{3}}$

Therefore, atomic packing factor

$$PF = \frac{\frac{8}{3}\pi r^3}{\frac{64}{3\sqrt{3}} r^3} = \frac{\sqrt{3}\pi}{8}$$

$$= 0.68 \text{ or } 68\%$$

The bcc structure also loosely packed Structure,

(iii) Face centred cubic structure (fcc) :-

In this structure, 8 atoms at eight corners and six atoms at the centre of six faces of a unit cell retain. Considering the atom at the face centre as origin, it can be observed that this face is common to two unit cells and there are twelve points surrounding it situated at a distance equal to half the face diagonal of the unit cell. Thus the co-ordination number of fcc lattice is twelve. The total number of atoms in fcc structure is $(\frac{1}{8}\times 8 + 6\times\frac{1}{2}) = 4$.

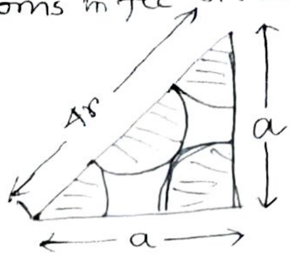


Fig (16)

Co-ordination number, $N = 12$

Lattice constant, $a = \frac{4r}{\sqrt{2}}$

Nearest neighbour distance, $2r = \frac{a}{\sqrt{2}}$

Number of atoms per unit cell, $n = 4$

Volume of all the atoms in a unit cell, $v = 4\times\frac{4}{3}\pi r^3$

Volume of unit cell, $V = a^3 = \frac{64r^3}{2\sqrt{2}}$

Atomic packing factor of FCC structure is

$$PF = \frac{v}{V}$$
$$= \frac{16}{3}\times\frac{\pi r^3 2\sqrt{2}}{64r^3} = \frac{\sqrt{2}\pi}{6} = \frac{\pi}{3\sqrt{2}} = 0.74 \text{ or } 74\%$$

This is a close pack structure.

(iv) Hexagonal close packed structure (hcp)

The hexagonal structure is shown in fig. (17). The unit cell contain one atom at each corner, one atom each at the centre of the hexagonal faces and three more atoms within the body of the cell. The centre atom of the hexagonal face touches three atoms in the layer below its plane, six atoms in its own plane and three atoms in the layer above its plane. Hence the co-ordination number is 12.

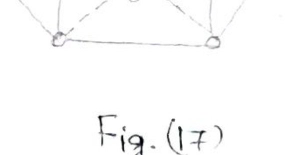


Fig. (17)

The atoms touch each other along the edge of the hexagon. Thus $a = 2r$

The top layer contain seven atoms. Each corner atom is shared by 6 surrounding hexagon cells and the centre atom is shared by 2 surrounding cells.

The total number of atoms in a unit cell is $12\times\frac{1}{6} + 2\times\frac{1}{2} +$

$= 2 + 1 + 3$

Calculation of c/a ratio for Hcp Structure:-

Let 'c' be the height of the unit cell and 'a' be its edge. The three ~~a~~ body atoms lie in a horizontal plane at $\frac{c}{2}$ from the orthocentres of alternate equilateral triangles at the top or base of the hexagonal cell. Three ~~atoms~~ three atoms just rest on the three atoms at the corners of the triangles.

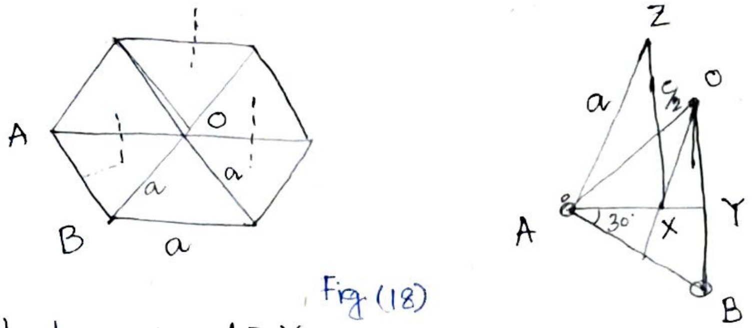


Fig. (18)

In the triangle ABY

$$\cos 30^\circ = \frac{AY}{AB}$$

$$\therefore AY = AB\cos 30 = \frac{\sqrt{3}\,a}{2}$$

$$AX = \frac{2}{3}AY = \frac{2}{3}\times\frac{\sqrt{3}}{2}a = \frac{a}{\sqrt{3}}$$

Now $AZ^2 = AX^2 + ZX^2$

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

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

$$\therefore \boxed{\frac{c}{a} = \sqrt{\frac{8}{3}}}$$

Volume of the unit cell:-

Area of the base = Six times the area of the triangle AOB

Area of the triangle, AOB $= \frac{1}{2}(BO)(AY)$

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

Thus area of the base $= 6\times\frac{\sqrt{3}}{4}a^2 = \frac{3\sqrt{3}}{2}a^2$

Volume of the cell, $V = \frac{3\sqrt{3}}{2}a^2c$

Calculation of Packing factor of hcp:-

Co-ordination number, $N = 12$

Lattice constant, $a = 2r$

Nearest neighbour, $2r = a$

Number of atoms per unit cell $= 6$

Volume of all atoms in a unit cell, $v = 6\times\frac{4}{3}\pi r^3$

$$= 8\pi\times\left(\frac{a}{2}\right)^3 = \pi a^3$$

Volume of the unit cell, $V = \frac{3\sqrt{3}}{2}a^2c$

$$\therefore \frac{c}{a} = \sqrt{\frac{8}{3}}$$

Packing factor, $(PF) = \frac{v}{V} = \frac{\pi a^3 \times 2}{3\sqrt{3}\,a^2c}$

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

$$= \frac{2\pi}{3\sqrt{3}} \times \sqrt{\frac{3}{8}}$$

$$= \frac{\cancel{2}\pi \times \sqrt{\cancel{3}}}{3\sqrt{\cancel{3}} \times \cancel{2}\sqrt{2}}$$

$$= \frac{\pi}{3\sqrt{2}} = 0.74 \text{ or } 74\%$$

HCP is an another close pack structure.

All fcc structures are ABCABC---- structure and all hcp structures are ABABAB---- structure.

Calculation of lattice Constant :-

If 'a' is the lattice constant and ρ the density of the crystal, then the mass of the unit cell is ρa^3.

If 'n' is the number of atoms or molecules in the unit cell, M is the atomic weight or molecular weight of the crystal, N the ~~avad a~~ Avagadro number then the mass of unit cell $= \frac{nM}{N}$

i.e. $\rho a^3 = \frac{nM}{N}$

or $\boxed{a = \left(\frac{nM}{\rho N}\right)^{1/3}}$