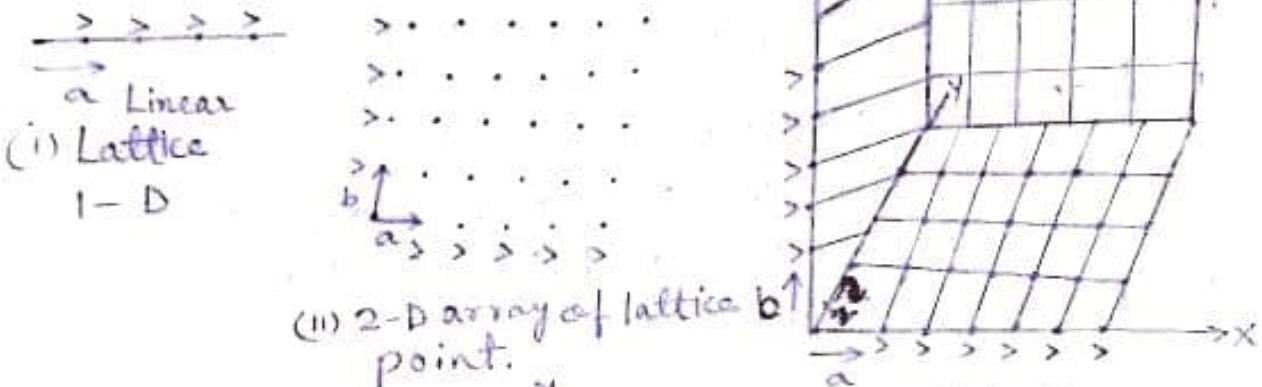
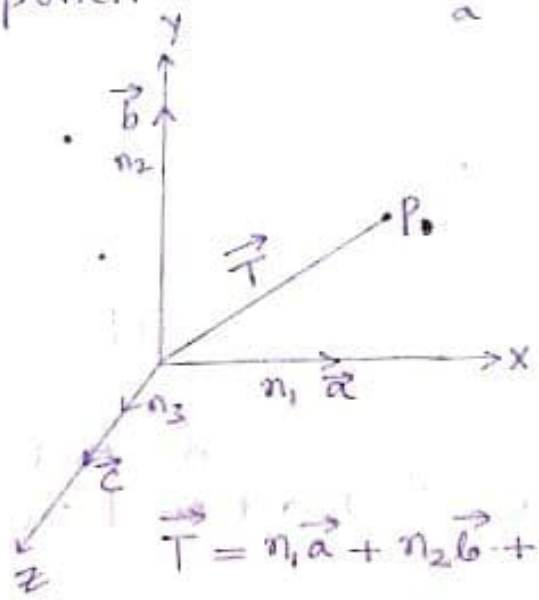
Crystal Translation vectors :-

In order to represent lattice points in space, a co-ordinate system is required. All the lattice points in space can be generated by translating three non-coplanar unit vectors. The three non-coplanar directions constitute a co-ordinate system.



Fig(iii)



$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}.$$

We know that a translation operator can be repeated an object infinite times in one direction and consequently, results in a linear array of repeated objects. A row of points repeated by a regular interval $\vec{a}$ is shown in fig (i) which is called a linear lattice. Now if the pattern in fig (i)

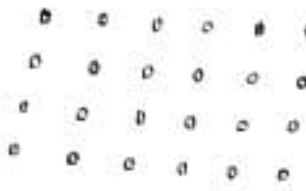
The Crystalline State :

The matter is usually regarded to exist in solid state or fluid state — the latter is subdivided into gaseous and liquid state. All the materials are composed of atoms and molecules. The solids are divided into two categories :—

(i) Crystalline and (ii) Amorphous.

(i) Crystalline :—

The solids are characterised by a perfect or nearly perfect periodicity of atomic structure. This geometric regularity of structure provides a simple conceptual picture of a crystal and helps a lot in gaining the knowledge of physical properties of the solid. In the crystalline state the atoms or molecules are in regular and geometric pattern.



(ii) Amorphous :—

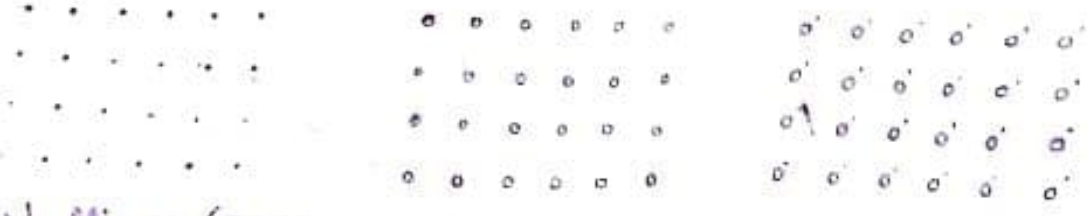
In amorphous solid though the atoms or molecules are strongly bonded at hardly there is any geometrical regularity or periodicity in the way in which the atoms are arranged in space. In such solids the atoms or molecules are not in regular and geometric pattern.

Unit Cell :-

The crystalline state refers to an infinite array of atoms or a group of atoms. The regularity in the arrangement or periodicity extends over the whole volume of a crystalline matter or crystal. The whole volume of a crystal can be constructed by moving a building block of the smallest exceptable size along its edges. This block consisting of atoms or a group of atoms is called a unit cell. A unit cell is the smallest geometric pattern, the repetation of which in three-D give the actual ~~crystal~~ crystal structures.

The basis and the Crystal Structure :-

(Since a point, being an infinitesimal small in a space, is imaginary, a lattice of points is an imaginary concept) If each atom in the crystal structure is replaced by a point, then we are left with an infinite array of points in space and the so called lattice is formed and each such point is called lattice points.



(i) Lattice or (Space lattice - 3D)

(ii) Basis ~~containing~~ 2D

(iii) Lattice + Basis = Crystal structure.

An infinite periodic array of points in space is called lattice [fig (i)]. In more general terms it is known as space lattice (3D). The arrangement of points defines the lattice symmetry. Generally atoms or groups of atoms are called basis [fig (ii)]. When

Table :- Bravais lattice and Crystal System :-

Crystal System	Bravais lattices	Symbols
Cubic	Simple	P
	Body-centred	I
	Face-centred	F
Tetragonal	Simple	P
	Body-centred	I
Orthorhombic	Simple	P
	Base-centred	C
	Body-centred	I
	Face-centred	F
Monoclinic	Simple	P
	Base-centred	C
Triclinic	Simple	P
Trigonal	Simple	P
Hexagonal	Simple	P

Space Lattices of Cubic Systems :-

There are three Bravais Lattices of cubic system as follows :—

(1) Simple cubic (or Primitive cubic) or cubic P-type lattice. In Simple cubic (SC) lattice, there are eight lattice points at the corners of the unit cell. Example :- KCl, and Po at certain temp^{r}.

(2) Face centred cubic or cubic F- lattice :- In addition to the lattice points at the eight corners it contains lattice points at the centre of each face. There is an extra lattice point at the centre of each face of the face-centred cubic (FCC) lattice

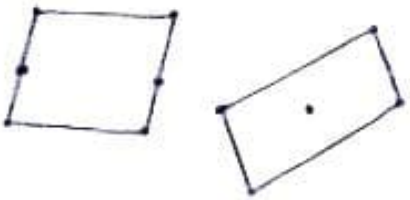
an atom or an identical group of atoms is attached to every lattice point, we obtain a crystal structure [fig (iii)]. i.e., lattice is a geometrical concept whereas crystal is a real thing.

Lattice + Basis = Crystal Structure.

Thus Crystal is not a lattice but it is a latticed array of atoms.

Difference between Unit Cell and Primitive Cell :-

A unit cell, in addition to an atom at its each corner, may or may not contain addition atom or atoms. But a primitive unit cell contains only one atom at its each corner.



(a) Unit Cells

(b) Primitive Unit Cells

From above we may conclude that all primitive cells are unit cells but all unit cells may or may not be primitive cells.

Lattice constant :-

The length a, b and c specifying the size of a unit cell are called lattice constants. For cubic crystal $a = b = c$ and a is called lattice constant.

Bravais Lattice :-

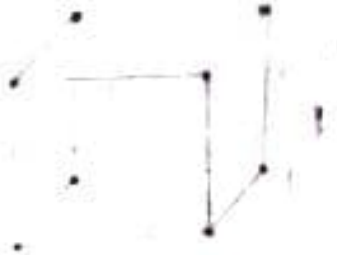
Bravais in 1884 proposed the concept of the space lattice. A space lattice is a mathematical concept which represents infinite number of points in space. such that the arrangement of points about a given point is similar to that about any other point.

There are 14 distinguishable ways in which points can be arranged in 3-D space. Therefore Bravais lattice are 14 number and belong to 7 crystal system. The 14 Bravais lattice and their names are listed in below diagram.

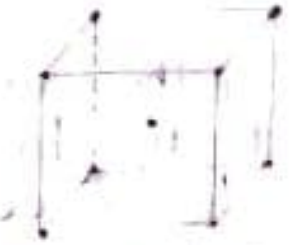
(i) Simple cubic (SC)

(ii) Body-centred cubic (BCC)

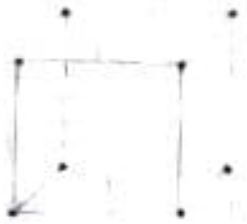
(iii) Face centred cubic (FCC)



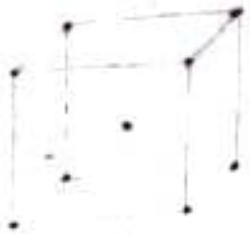
(iv) Simple tetragonal (ST)



(v) Body Centred tetragonal (BCT)



(vi) Simple orthorhombic (SOR)



(vii) Body-centred orthorhombic

(viii) Face centred orthorhombic

For example, take a plane having the intercept of length 2a, b and 2c with the three Crystal axes. In order to find its Miller indices first take the reciprocals of 2, 1 and 2 getting $\frac{1}{2}$, 1, $\frac{1}{2}$ and then find the integers that are in the same ratio as $\frac{1}{2}$, 1, $\frac{1}{2}$. This gives the Miller indices (1 2 1).

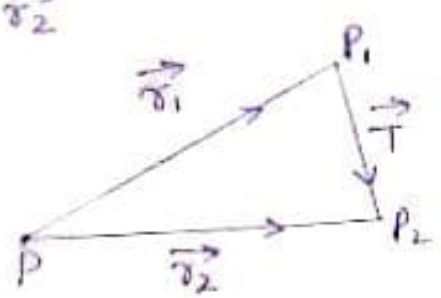
is repeated at an interval b in a direction other than that of repetition in fig (i), the two dimensional array of points is obtained as shown in fig (ii). Finally, if the plane pattern of fig (ii) having repetition intervals a and b, is repeated by a third non-coplanar translation c; a three dimensional space lattice is generated as shown in fig (iii)

If the translations $\vec{a}$, $\vec{b}$ and $\vec{c}$ are regarded as vectors and the three translation direction are selected as crystallographic axes x, y and z respectively w.r.t. any lattice point chosen as origin, then the location of any other lattice point (P) can be defined w.r.t this origin by

$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c},$$

where n_1, n_2 and n_3 are arbitrary integers. $\vec{a}$, $\vec{b}$ and $\vec{c}$ are called fundamental vectors while $\vec{T}$ is called Crystal Translation Vector.

A proper description of the subject may be carried out by referring to the three dimensional space lattices. Draw a vector $\vec{T}$ connecting two lattice points P_1 and P_2 as shown in figure represented by the position vectors $\vec{r}_1$ and $\vec{r}_2$ respectively. Then the vector $\vec{T}$ is given by the relation



$$\vec{r}_2 = \vec{r}_1 + \vec{T}$$

But $\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$

$$\therefore \quad \vec{r}_2 = \vec{r}_1 + n_1\vec{a} + n_2\vec{b} + n_3\vec{c}.$$

example :- Cu, Ni, Au, Ag Crystals.

(3) Body-centred cubic or cubic I lattice :- In body centred cubic (BCC) lattice, there is one additional lattice point situated at the body centre besides eight lattice points situated at the eight corners. Thus there is an extra lattice point at the body centre of the unit cell.

example :- Li, Na, K, Cr crystals

Calculation of Number of atoms per unit cell :-

(1) Simple cubic (SC) lattice :- Every lattice point in SC lattice situated at the corner of the unit cell is shared by eight unit cells and hence its contribution to each cell is $\frac{1}{8}$.

Total contribution of eight corners of the SC lattice is $\frac{1}{8} \times 8 = 1$.

Thus, for an SC lattice there is one lattice point per unit cell.

(2) Face-centred cubic (FCC) lattice :- There are eight lattice points at the eight corners of the FCC lattice and contribution of these eight lattice points to the unit cells is $\frac{1}{8} \times 8 = 1$.

Moreover, there are six faces of the unit cell each atom of which belongs to two unit cells. So, the contribution of these six lattice points to the unit cell is $\frac{1}{2} \times 6 = 3$.

∴ Total number of lattice points per FCC cell is = 1+3 = 4

(3) Body-centred cubic (BCC) :— Here there are eight lattice points at the eight corners of the unit cell and each is a number of eight unit cells. In addition, there is one lattice point at the body centre. So, the total number of lattice points per BCC unit cell

$\frac{1}{8} \times 8 + 1 = 2$.

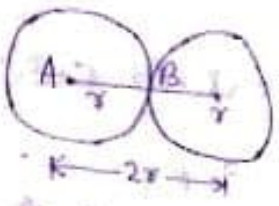
Co-ordination number :- (CN) :

For a particular lattice, co-ordination number is defined as the number of equivalent nearest neighbours to a particular atom in the crystal lattice.

Nearest neighbours distance (a) :-

It is defined as the distance between the centres of two nearest neighbouring atom in a crystal.

As shown in the figure the nearest neighbour distance is 2r.



Atomic radius (r) :—

Atomic radius is defined as half of the distance between nearest neighbour atom in the crystal.

Here, the atoms are supposed to be

Spherical in size and any two neighbouring atoms touch each other.

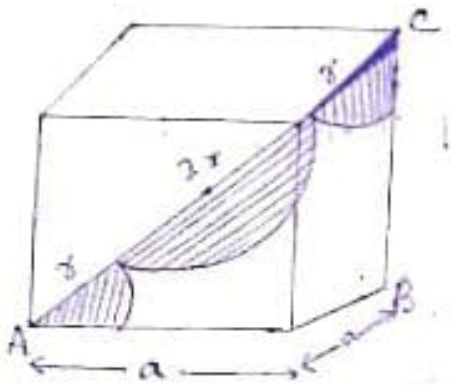
(i) SC lattice :-

As shown in the fig. AB represent the radius r of an atom and $r = \frac{1}{2} \times$ nearest neighbour distance

$$= \frac{1}{2} \times a = a/2.$$

∴ The nearest neighbour distance $d = 2r = 2 \times a/2 = a$

(ii) BCC lattice :-



Geometry of a BCC unit cell

In fig. a BCC unit cell is shown where $AB^2 = a^2 + a^2$

∴ $AB = \sqrt{2}a$ and $AC^2 = (\sqrt{2}a)^2 + a^2 = 3a^2$.

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

∴ atomic radius $r = \frac{\sqrt{3}a}{4}$ $(\because 4r = \sqrt{3}a)$

So the atomic radius of a BCC crystal is $r = \frac{\sqrt{3}a}{4}$

∴ The nearest neighbour distance $d = 2r = \frac{\sqrt{3}a}{2}$

Miller discovered a method to designate a plane in a crystal using three numbers h, k and l known as Miller indices.

"Miller indices are the 3 smallest possible integers which have the same ratios as the reciprocals of the intercepts of the plane concerned on the 3 axes.

Indices of a Lattice Direction and Lattice Plane:-

The exercise of describing a crystal structure essentially amounts for locating the position of different atoms in the unit cell. But the study of many physical properties of crystals becomes more meaningful and complete with the knowledge of direction and various atomic plane visualized within their crystalline medium. These are identified by using the index system discussed below:-

Indices of a lattice direction:-

A vector is drawn along (or parallel to) the desired direction from the origin fixed for the axes system. The components of these vectors along the crystal axes are determined and reduced to smallest integers. This integers when written within square brackets represents the indices of the direction. A bar on the index means that the respective component of the vector is negative. 23/5/21

Indices of a Lattice Plane :-

Every crystal plane is identified by its orientation which is characterized by planes intercepts with the crystal axes. The eqⁿ of a plane having intercepts p, q and r with x, y and z axes is given by

$$\frac{x}{p} + \frac{y}{q} + \frac{z}{r} = 1 \longrightarrow (1)$$

The form of this eqⁿ has been exploited by Miller to develop an index system, for, whom the indices are named Miller indices. The Miller Indices of a plane are determined by the following procedure.

(i) Find the intercepts on the three crystallographic axes OX, OY and OZ.

(ii) Note their reciprocals.

(iii) Clear the fraction.

Let the intercepts of a plane with a, b and c measure as pa, qb and rc respectively. Take their reciprocal set $\frac{1}{p}, \frac{1}{q}, \frac{1}{r}$ to the three integers h, k, l having the same ratio as $\frac{1}{p}, \frac{1}{q}, \frac{1}{r}$. This set of indices when written in parenthesis as (hkl) gives the miller indices of the plane.

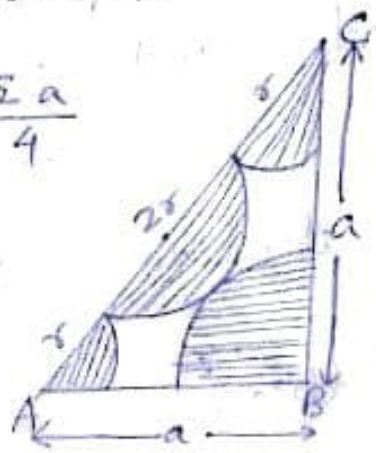
(iii) FCC lattice:-

In fig. an FCC unit cell whose face diagonal is AC.

Face diagonal, $AC = \sqrt{2}a = 4r$

atomic radius, $r = \frac{\sqrt{2}a}{4}$

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



The nearest neighbour distance $d = 2r = \frac{a}{\sqrt{2}}$

Lattice Planes and Miller Indices:-

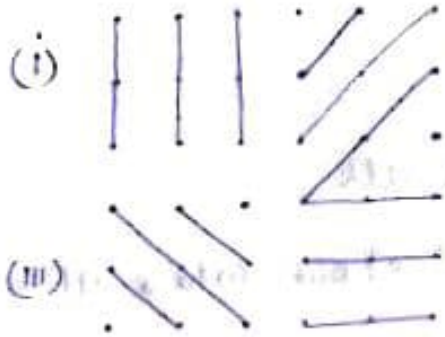
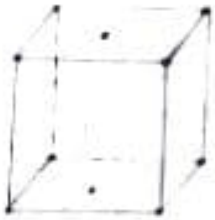


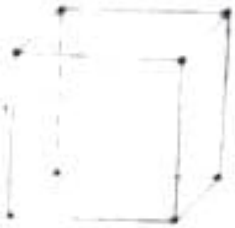
Fig:- Set of lattice planes

A crystal lattice may be consider as an aggregate of a set of parallel equidistance planes passing through the lattice points. These sets of parallel planes are called lattice planes which can be chosen in a number of ways like (i), (ii), (iii) and (iv) as shown in the figure.

(X) Simple monoclinic



(XI) Base centred monoclinic



(XII) Triclinic

(XIII) Trigonal

(XIV) Hexagonal

Table Crystal System :-

Crystal System	Lattice constants	α, β, γ	Example
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	NaCl, CaF_2, $NaClO_2$
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	$NiSO_4$, SnO_2
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = 90° = \gamma$	KNO_3, $BaSO_4$, $MgSO_4$
Monoclinic	$a \neq b \neq c$	$\alpha = \beta = 90°, \gamma \neq 90°$	Na_2SO_4, $FeSO_4$
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	$CuSO_4$, $K_2Cr_2O_7$
Trigonal	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	$CaSO_4$
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	SiO_2, AgI

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