UNIT-I

CRYSTAL STRUCTURE

Elements and their chemical combinations are found to occur in three states i.e solids, liquids and gases. 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 atom 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 solids may be sub-divided into single crystals and polycrystalline 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 seperated by well-defined boundaries. The small crystallites are known as grains and the boundaries as grain boundaries. Most of the metals and ceramics exhibit polycrystalline structure

The non-crystalline or amorphous solids are characterized by the completely random arrangement of atoms or molecules. The periodicity, if at all present, extends up to a distance of a few atomic diameters only. In other words, these solids exhibit short range order. such type of materials are formed when the atom do not get sufficient time to undergo a periodic arrangement. Glass is an example of amorphous material. Most of the plastics and rubbers are also amorphous.

"The science which deals with the study of geometrical forms and physical properties of crystalline solid is called crystallography."

The study of crystallography is necessary to understand the strong correlation between the structure of material and its physical properties.

* Crystal Lattice and Translation vectors

A crystal is a three dimensional body, which is made up of regular and periodic three dimensional patterns of atoms or molecules in space. The crystal structure can be described in terms of a geometrical concept called space lattice. The space lattice is defined as

"An arry of points in space such that the environment about each point is the same."

similarly, the three dimensional lattice is defined as

"An ~~array~~ infinite array of points in three dimensions in which every point has an identical environment, as any other point in the array."

The term identical environment or surroundings means that the lattice has the same appearance when viewed from a point r in the lattice as it has when viewed from any other point r' with respect 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 T given by

$$T = n_1\bar{a} + n_2\bar{b} + n_3\bar{c} \quad \text{------} \quad (1)$$

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

$$r' = r + T$$

$$= r + n_1\bar{a} + n_2\bar{b} + n_3\bar{c} \quad \text{-----} \quad (2)$$

In a perfect lattice eq.(2) holds good, i.e point r' can be obtained from r by the application of the operation (1). However, in an imperfect lattice, it is not possible to find $\bar{a}$, $\bar{b}$ and $\bar{c}$ such that an arbitrary choice of n_1, n_2 and n_3 makes r' identical to r.

The translation vectors $\bar{a}$, $\bar{b}$ and $\bar{c}$ are also called the crystal axes or basis vectors.

consider a part of a two-dimensional lattice as shown in below Fig. 1

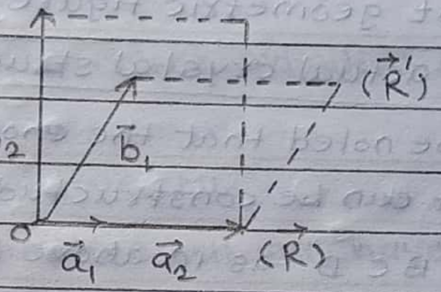


Fig. 1

The translation vectors $\bar{a}$ and $\bar{b}$ can be chosen in a number of ways. Two such possibilities are shown in this figure where two sets $\bar{a}_1$, $\bar{b}_1$ and $\bar{a}_2$, $\bar{b}_2$ of translation vectors are drawn.

* Unit Cell

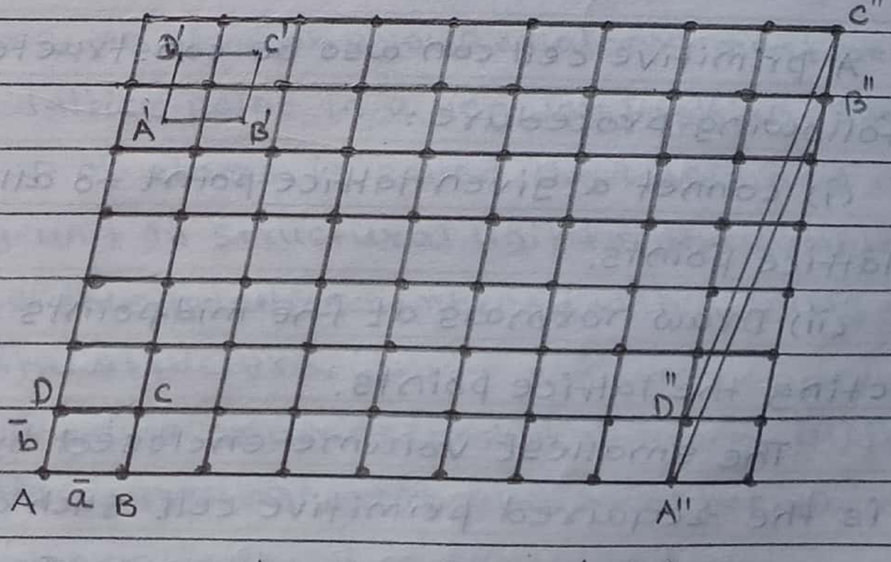


Fig. 1 Unit cell and crystal lattice

The parallelograms formed by the translation vectors may be regarded as building blocks for constructing the complete crystal lattice as shown in Fig. 1. These are known as unit cells of the lattice.

The parallelopiped formed by using the primitives $\bar{a}$, $\bar{b}$, $\bar{c}$ as concurrent edges is called unit cell of the space lattice. The angles between primitives (b, c), (c, a) and (a, b) are denoted by α, β and γ respectively

The unit cell is defined as

"The smallest geometric figure, the repetition of which gives the actual crystal structure".

It should be noted that the choice of a unit cell is not unique but it can be constructud in a number of ways as $A'B'C'D'$ or $A''B''C''D''$ as in above Fig. 1

<I> primitive unit cell

primitive unit cell is the smallest volume cell. All the lattice points belonging to a primitive cell lie at its corners. Therefore, the effective number of lattice points in a primitive unit cell is one.

➡ The volume of the primitive cell is given by

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

A primitive cell can also be constructed using the following procedure:

(i) connet a given lattice point to all the nearby lattice points.

(ii) Draw normals at the mid-points of lines connecting the lattice points.

The smallest volume enclosed by the normals is the required primitive cell. Such a cell is called Wigner-Seitz cell as is shown in Fig. 2

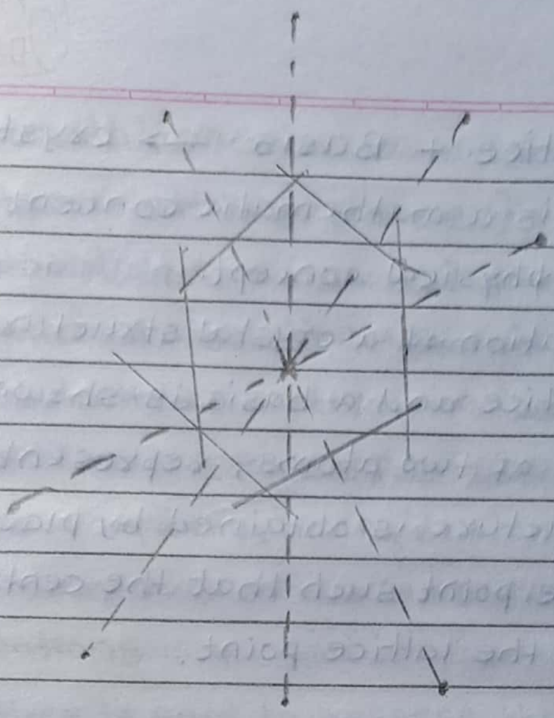


Fig.2 Wigner-Seitz primitive cell

⟨II⟩ Non-primitive cell

A non-primitive cell may have the lattice points at the corners as well as at other locations both inside and on the surface of the cell and, therefore, the effective number of lattice points in a non-primitive cell is greater than one.

* Basis

The crystal structure is always described in terms of atoms rather than points. Thus to obtain a crystal structure, an atom or group of atoms must be placed on each lattice point in a regular fashion. Such an atom or a group of atoms is called the basis and acts as a building unit or structural unit for the complete crystal structure. Thus a lattice combined with a basis generates the crystal structure

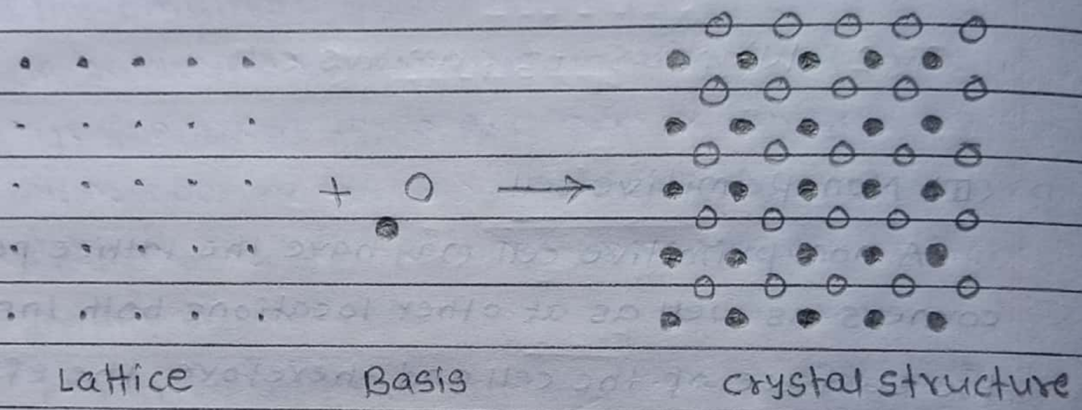
"A basis is an assembly of atoms identical in composition, arrangement and orientation."

Mathematically, it is expressed as

space lattice + Basis → crystal structure

Thus, a lattice is a mathematic concent and the crystal structure is a physical concept.

The generation of a crystal structure from a two-dimensional lattice and a basis is shown in Fig.1. The basis consists of two atoms, represented by ○ and ●. The crystal structure is obtained by placing the basis on each lattice point such that the centre of the basis coincides with the lattice point.



* Symmetry operations

A symmetry operation is that which transforms the crystal to itself, i.e. a crystal remains invarient under a symmetry operation. These operations are

<I> translation

<II> rotation

<III> reflection and

<IV> inversion

The translation operation applies to lattices only while all the remaining operations and their combinations apply to all objects and are collectively known as point symmetry operations. The inversion operation is applicable only to three dimensional crystals.

⟨I⟩ Translations

The translation symmetry follows from the orderly arrangement of a lattice. It means that a lattice point r, under lattice translation vector operation T, gives another point r' which is exactly identical to r, i.e.

$$r' = r + T$$

where $T = n_1 \bar{a} + n_2 \bar{b} + n_3 \bar{c}$

⟨II⟩ Rotations

A lattice is said to possess the rotation symmetry if its rotation by an angle θ about an axis transforms the lattice to itself. Also, since the lattice always remains invarient by a rotation of 2π, the angle 2π must be an integral multiple of θ, i.e

$$n\theta = 2\pi$$

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

The factor n takes integral values and is known as multiplicity of rotation axis. The possible values of n which are compatible with the requirement of translation symmetry are 1, 2, 3, 4 and 6 only. Thus for example, for n equal to 6, θ is 60° which means that the lattice repeats itself with a minimum rotation of 60°. such a rotation is shown in below Fig. 1.

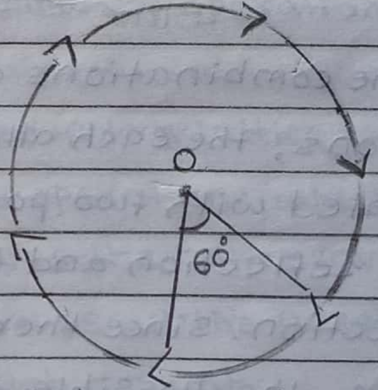


Fig. 1. Six-fold rotation about the point O in two dimension

Regular hexagon is an example of such lattice. A rotation corresponding to the value of n is called n-fold rotation. A two-dimensional square lattice has 4-fold rotation symmetry. It may be noted that a rotation axis may or may not pass through a lattice point. The fact that 5-fold rotation is not compatible with translation symmetry operation and that only 1, 2, 3, 4 and 6-fold rotations are permissible.

<III> Reflections

A reflection symmetry divides the lattice into two identical halves which are mirror images of each other. The plane (or line) which divides the lattice is represented by m. The reflection symmetry of a notched wheel is illustrated in Fig. 1

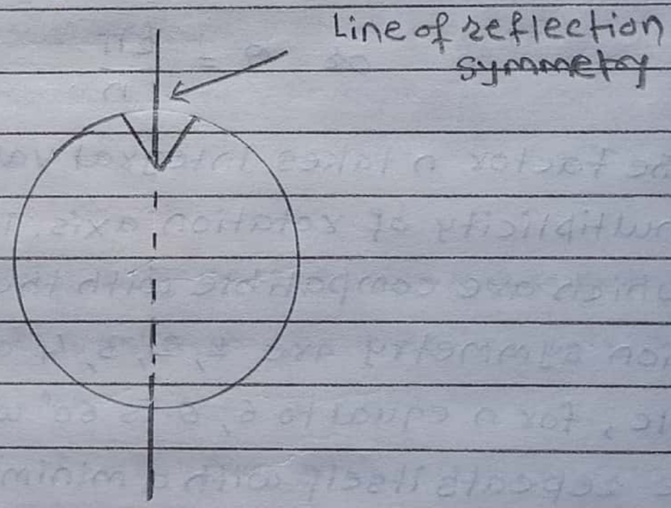


Fig. 1 Reflection symmetry of a notched wheel about a line

considering the combinations of reflections with allowed rotations, the each allowed rotation axis can be associated with two possibilities: one is rotation with reflection and the other rotation without reflection. Since there are five allowed rotations axes, the possible number of such combinations is 10. These are designated as

1, 1m, 2, 2mm, 3, 3m, 4, 4mm, 6, 6mm

where the numerals represent the type of rotation axis, the first m represents a plane (or line) parallel to the rotation axis and the second m refers to another plane (or line) ⊥r to the rotation axis.

<IV> Inversions

Inversion is a point operation which is applicable to three-dimensional lattices only. This symmetry elements implies that each point located at r relative to a lattice point has an identical point located at $-r$ relative to the same lattice point. In other words, it means that the lattice possesses a centre of inversion denoted by $\bar{1}$.

* Point Groups and Space Groups

→ Point Groups

There are mainly four types of symmetry operations, 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.

"A point group in a lattice is defined as the collection of symmetry operations which when applied about a lattice point leaves the lattice invarient."

In point groups all the possible symmetry elements must pass through a point.

In two-dimensional space, rotation and reflection are the only point operations. Their combinations yield 10 different point groups designated as 1, 1m, 2, 2mm, 3, 3m, 4, 4mm, 6 and 6mm. In three-dimensional space the situation is complicated due to the presence of additional point operations such as inversion. Thereare a total of 32 point groups in a three-dimensional lattice.

→ Space Group

" The group of all the symmetry elements of a crystal structure is called" space group."

It determines the symmetry of a crystal structure as a whole. There are 17 and 230 distinct space groups possible in two and three dimensions respectively.

→ The symmetry of a crystal structure is specified completely when the space group is known.

→ The space group is characterized by Bravais lattice and by the location of the point group and other symmetry elements in a unit cell.

→ The space group through its symmetry elements determines the positions of equivalent points within the unit cell.

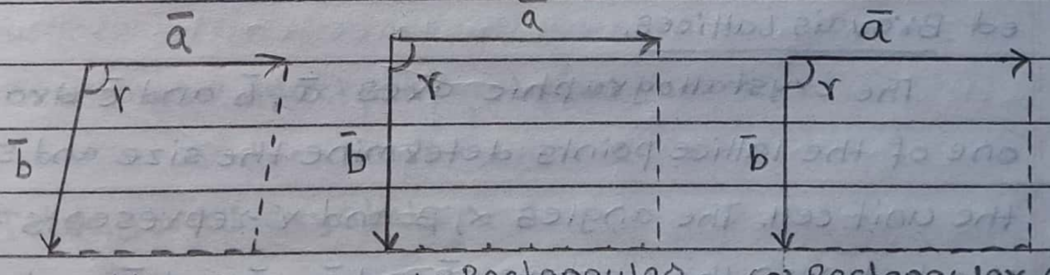
→ For a crystal structure specified by a particular space group if only one point in a cell is occupied, it is necessary that all equivalent points will be occupied by identical atoms or molecules.

* Types of Lattices

The number of point groups in two and three dimensions are 10 and 32 respectively. These point groups form the basis for construction of different types of lattices. only those lattices are permissible which are consistent with the point group operations. such lattices are called Bravais Lattices. It can be stated that 10 and 32 point groups in two and three dimensions produce only 5 and 14 distinct Bravais lattices respectively. These Bravais lattices further becomes part of 4 and 7 distinct crystal systems respectively.

⟨I⟩ Bravais Lattices in Two-Dimensions

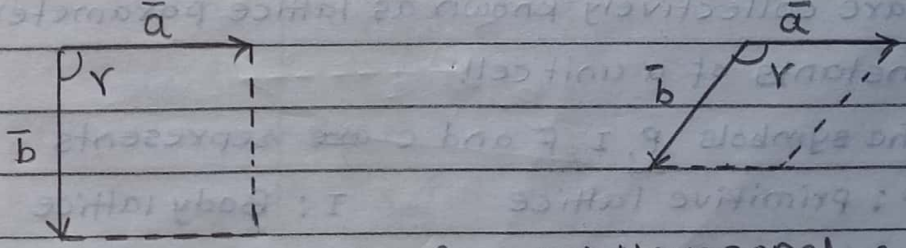
The four crystal systems of two-dimentional space are (1) oblique, (2) Rectangular, (3) square, and (4) Hexagonal. The rectangular crystal system has two Bravais lattices, (i) rectangular primitive (ii) rectangular centred. In all, there are five Bravais lattices given in below table along with the corresponding point groups. These lattices are shown in below Fig. 1.



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

(b) Rectangular ~~Primitive~~ $a \neq b$ $\gamma = 90^\circ$

(c) Rectangular centred $a \neq b$ $\gamma = 90^\circ$



(d) square $a=b$, $\gamma = 90^\circ$

(e) Hexagonal $a=b$, $\gamma = 120^\circ$

Fig. 1 Bravais Lattices in Two-dimensions

Sr. No	crystal system	unit cell characteristics	Bravais Lattice	conventional unit cell
1	oblique	$a \neq b$, $\gamma \neq 90^\circ$	oblique	parallelogram
2.	Rectangular	$a \neq b$, $\gamma = 90^\circ$	1. Rectangular primitive 2. Rectangular centred	Rectangle
3	square	$a = b$, $\gamma = 90^\circ$	square	square
4	Hexagonal	$a = b$, $\gamma = 120^\circ$	Hexagonal	60° Rhombus

⟨II⟩ Bravais Lattices in Three-Dimensions

Space lattices can be classified according to their symmetry. In 1948, Bravais showed that fourteen (14) classes of lattices were sufficient in three dimensions. According to Bravais, there are fourteen types of space lattices in the seven systems of crystals, which are called Bravais Lattices.

The crystallographic axes $\bar{a}$, $\bar{b}$ and $\bar{c}$ drawn from one of the lattice points determine the size and shape of the unit cell. The angles α, β and γ represents the angles between the vectors $\bar{b}$ and $\bar{c}$, $\bar{c}$ and $\bar{a}$ and $\bar{a}$ and $\bar{b}$ respectively. The lengths a, b and c and angles α, β and γ are collectively known as lattice parameters or lattice constants of a unit cell.

The symbols P, I, F and C ~~are~~ represents

P : primitive lattice

I : Body lattice

F : Face lattice

C : Base lattice

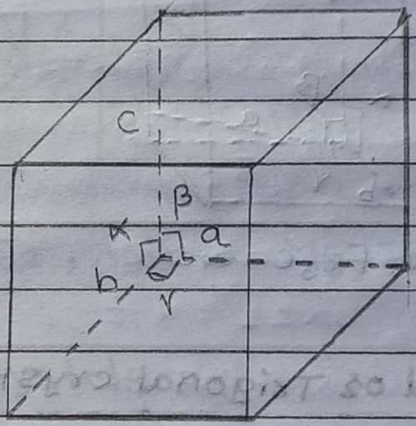
The seven crystal systems are

1. Cubic
2. Tetragonal
3. Orthorhombic
4. Rhombohedral or Trigonal
5. Hexagonal
6. Monoclinic
7. Triclinic

1. Cubic crystals

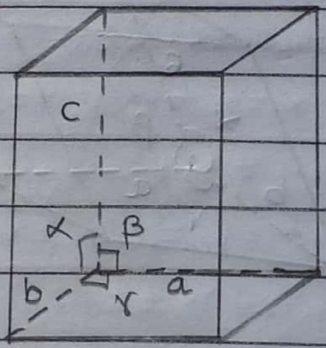
In this crystal all the three lengths of the unit cell are equal and right at right angles to each other.

i.e $a = b = c$ and $\alpha = \beta = \gamma = 90°$



Examples : NaCl, CaF, $NaClO_2$ etc

2. Tetragonal crystals



In this crystal the two lengths of the unit cell are equal while third one is longer. The three axes are $\perp$r.

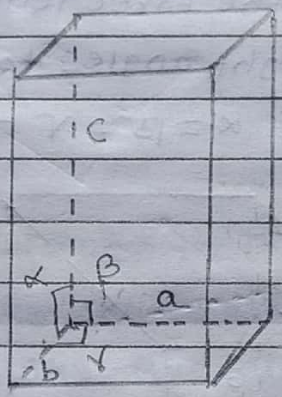
i.e $a = b \neq c$ and $\alpha = \beta = \gamma = 90^\circ$

Examples: $NiSO_4$, SnO_2 etc.

3. Orthorhombic crystals

In this crystal the lengths of unit cell are different. But three axes are right angles to each other

i.e $a \neq b \neq c$ and $\alpha = \beta = \gamma = 90^\circ$

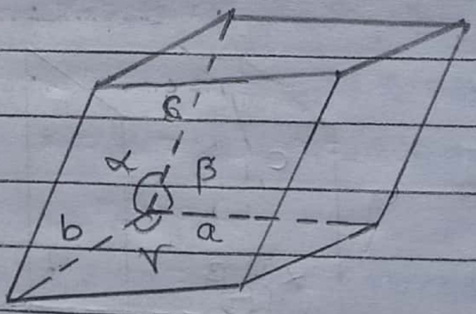


Examples: Ga, Fe_3C etc

4. Rhombohedral or Trigonal crystals

In this crystals all the three lengths of the unit cell are equal in length and they are equally inclined to each other at an angle other than 90°.

i.e $a = b = c$ and $\alpha = \beta = \gamma \neq 90^\circ$

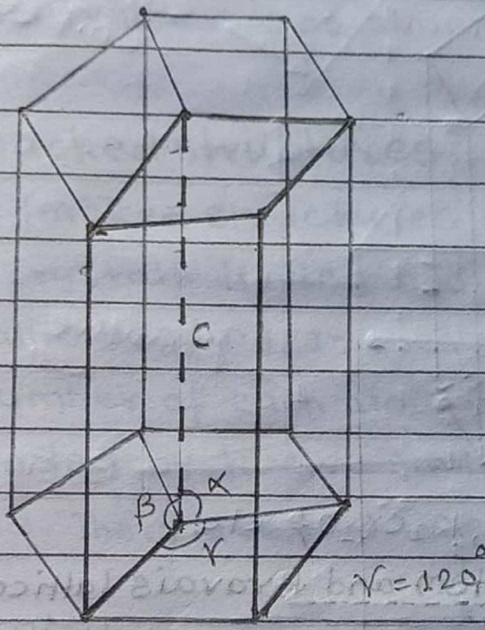


Examples: As, Sb, Bi

5. Hexagonal crystal

In this crystal the two axes of the unit cell are equal in length in one plane at 120° with each other and third axis is ⊥r to this plance

i.e. $a = b \neq c$ and $\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$

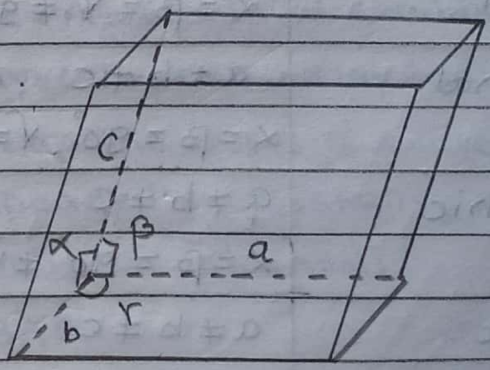


Examples : SiO_2 , AgI ~~etc~~ Mg, Zn, Cd etc

6. Monoclinic crystals

In this crystal the lengths of unit cell are different. Two axes are at right angles and third is obliquely inclined.

i.e $a \neq b \neq c$ and $\alpha = \beta = 90^\circ \neq \gamma$.

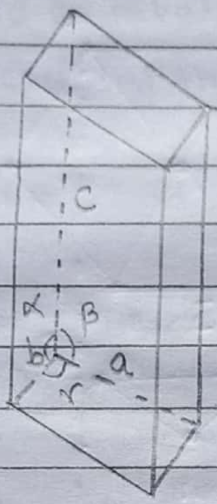


Examples : $CaSO_4 \cdot 2H_2O$ gypsum.

7. Triclinic crystal

In this crystal the lengths of unit cell are different and oblique to each other

i.e $a \neq b \neq c$ and $\alpha \neq \beta \neq \gamma \neq 90^\circ$



Examples: $CuSO_4$, $K_2Cr_2O_7$ etc.

Table - crystal system and Bravais lattices in 3D

Sr No.	Crystal System	Lattice parameters	Lattice symbols	Examples
1	Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	P, I, F	Cu, Ag, Fe Na NaCl CsCl
2	Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma \neq 90^\circ$	P, I	β-Sn, TiO_2
3.	orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	P, C, F, I	Ga, Fe_3C
4	Rhombohedral or Trigonal	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	P	As, Sb, Bi
5.	Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	P	Mg, Zn, Cd, NiAs
6.	Monoclinic	$a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma$	P, C	$CaSO_4 \cdot 2H_2O$ (gypsum)
7.	Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$	P	$K_2Cr_2O_7$

* Simple Crystal Structure

The basic crystal structures are either monoatomic or contain simple basis. These include -

(i) close-packed structures
[Hexagonal closed packed or face-centred cubic]
(ii) Loose-packed structures
[Body centred cubic or simple cubic]

(I) Close-packed structures

Close-packed structures are mostly found in monoatomic crystals having non-directional bonding, such as metallic bonding. In these structures, the co-ordination number of each atom is 12, i.e. each atom is surrounded by twelve similar and equal sized neighbours. There are two types of ~~closed~~ closed packed structures:

(i) Hexagonal close-packed (HCP) structure
(ii) Face-centred cubic (FCC) structure

(I) Hexagonal Close-Packed Structure (HCP)

Consider a layer of similar atoms with each atom surrounded by six atoms in one plane. Another similar layer B can be placed on top of layer A such that the atoms of the layer B occupy the alternate valleys formed by the atoms of layer A. If a third similar layer is placed on top of the B-layer in such a way that the atoms of B-layer exactly overlap the atoms of A-layer and this type of stacking is repeated successfully, the following layered arrangement is obtained:

... ABABAB ...

This type of stacking is called hcp stacking and the structure is known as hexagonal close-packed structure. The name corresponds to the shape of the conventional unit cell which is hexagonal and is shown in Fig. 1.

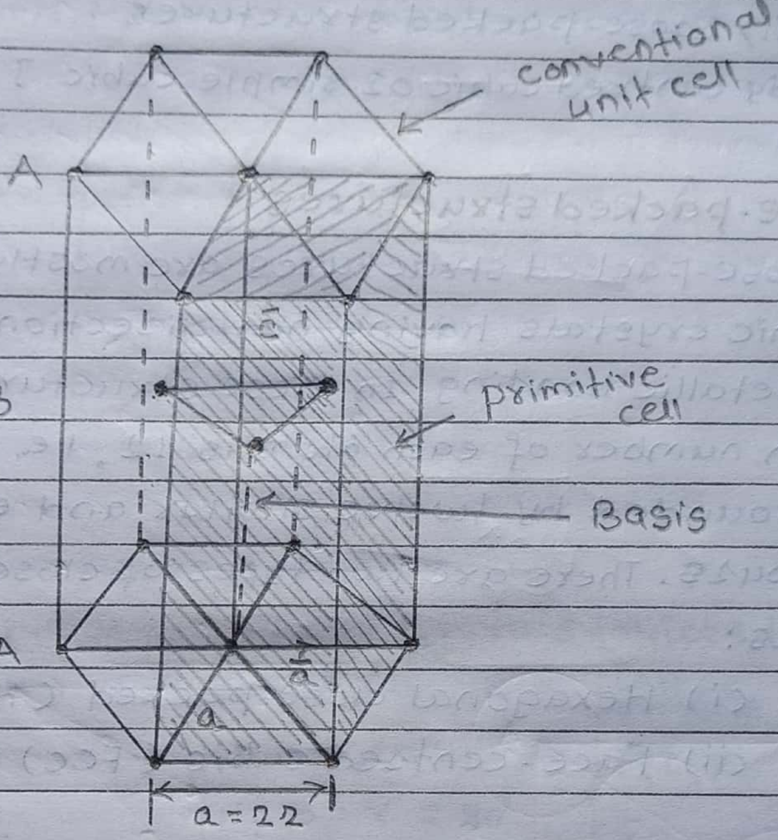


Fig. 1 conventional and primitive cells of hexagonal close-packed structure.

There are twelve atoms located at the corners, two at the centres of the basal planes, and three completely inside the hexagon forming a part of the B-layer. The effective number of atoms in a unit cell is

$$12\left(\frac{1}{6}\right) + 2\left(\frac{1}{2}\right) + 3 = 2 + 1 + 3$$
$$= 6$$

The interatomic distance for the atoms within a layer is a. The distance between the two adjacent layer is $c/2$, c being the height of the unit cell. For an ideal hcp structure, $c = 1.633a$.

The packing fraction, f, is defined as the ratio of the volume occupied by the atoms present in a unit cell to the total volume of the unit cell. It is also refered as the packing factor or packing efficiency of the unit cell. From the primitive cell, we find

$$f = \frac{2\left(\frac{4}{3}\right)\pi r^3}{a(a\sin 60^\circ)c}$$

where r is the atomic radius. Using $c = 1.633a$ and $a = 2r$, we get

$$\therefore f = \frac{2(4/3)\pi r^3}{1/2\sqrt{3}a^2c}$$

$$= \frac{8/3\,\pi r^3}{\sqrt{3}/2 \cdot 1.633 \times a^3} = \frac{16}{3\sqrt{3}} \frac{\pi r^3}{(2r)^3}$$

$$= \frac{16}{3\sqrt{3}} \frac{\pi r^3}{8r^3(1.633)} = \frac{2\pi}{3\sqrt{3}(1.633)}$$

$$= 0.74$$

Thus, in an ideal hcp structure, 74% of the total volume is occupied by atoms.

Metals like Mg, Zn, Cd, Ti, Be, etc exhibit this type of structure.

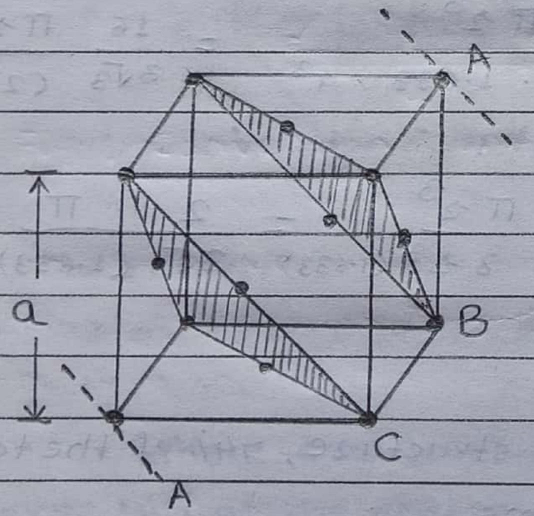
~~<II> Facecentred~~

<II> Face-Centred Cubic (FCC) Structure

In FCC structure, the stacking of first two layers A and B is similar to that of HCP structure. The difference arrises in the third layer which does not overlap the first layer. The atoms of the third layer occupy the positions of those valleys of the A-layer which are not occupied by the B-layer atoms. The third layer is designated by the letter C. The fourth layer exactly overlaps the first layer and the sequence is repeated. Thus FCC structure is represented by the following stacking sequence:

--- ABCABCABC ---

The conventional unit cell is face-centred cubic and is shown in Fig 1(a).



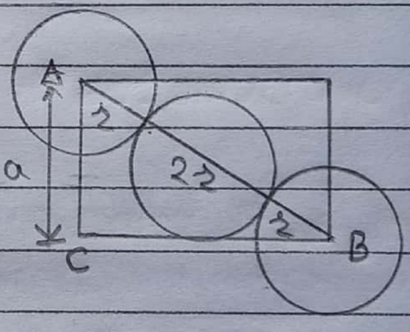


Fig 1 (b)

Fig. 1 (a) conventional unit cell of FCC structure

The atoms touch one another along the face diagonals. The length of the cube edge, a and the atomic radius ~~a~~ 'r' are related to each other as

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

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

Hence volume of the cube $= \left(\frac{4}{\sqrt{2}} r\right)^3$

Number of spheres in one unit cell

$$= \frac{6}{2} + \frac{8}{8} = 3 + 1$$

$$= 4$$

$\therefore$ Packing fraction $= \dfrac{\text{complete volume of spheres}}{\text{volume of cube}}$

$$= \frac{4\left(\frac{4}{3}\pi r^3\right)}{\left(\frac{4}{\sqrt{2}} r\right)^3}$$

$$= \frac{4 \cdot \frac{4}{3}\pi r^3}{\frac{4 \times 4 \times 4}{2\sqrt{2}} r^3} = \frac{\pi}{3 \times 2/\sqrt{2}}$$

$$= \frac{\pi\sqrt{2}}{6}$$

$$= 0.74$$

$\therefore$ $f = 0.74$ or 74%

Thus the packing fraction of FCC structure is exaclty the same as that of HCP structure which is expected because of the close-packed nature of both the structures. Also, the co-ordination number of each atom is 12. Elements having face-centred cubic structure are Cu, Ag, Au, Ca, Al, Pb, etc.

(II) Loose-Packed Structures

A loose-packed structure is that in which the co-ordination number of an atom is less than 12 or the packing fraction is less than 0.74. Among the various possible loose-packed structures, the most common and the simplest are the body-centred cubic (BCC) and the simple cubic (SC) structures.

(I) Body-Centred Cubic structure (BCC)

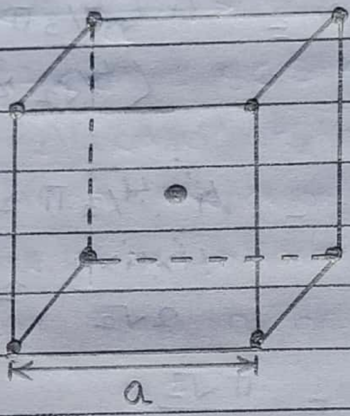


Fig. 1 Conventional unit cell of BCC structure.

The conventional unit cell of BCC structure is non-primitive and is shown in above Fig 1. This unit cell is cubic with an atom located at each corner and an atom in the centre of the cube. This structure is not close-packed since each atom has only eight neighbours. The atoms are in contact along body diagonals.

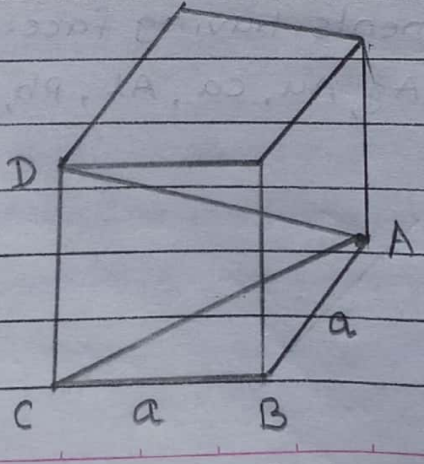


Fig. 2 Body centred cubic structure

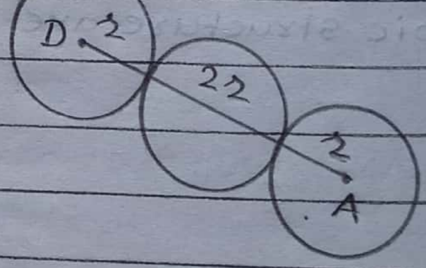


Fig. 3

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

$= 1 + 1 = 2$

In ΔABC, (from Fig. 2)

$$AC^2 = AB^2 + BC^2$$
$$= a^2 + a^2 = 2a^2$$
$$\therefore AC^2 = 2a^2$$

In ΔACD,

$$AD^2 = AC^2 + CD^2$$
$$= 2a^2 + a^2$$
$$\therefore AD^2 = 3a^2$$

If r is the atomic radius, then

$$AD = r + 2r + r = 4r$$
$$\therefore 4r = \sqrt{3}a$$
$$r = \frac{\sqrt{3}}{4}a$$

Packing fraction $= \frac{\text{Volume of all atoms in unit cell}}{\text{Volume of unit cell}}$

$$= \frac{2 \times 4/3 \pi r^3}{a^3}$$
$$= \frac{2 \times 4/3 \pi \left(\sqrt{3}/4\, a\right)^3}{a^3}$$
$$= \frac{8\pi}{3a^3} \times \frac{3\sqrt{3}}{64} a^3 = \frac{\sqrt{3}\pi}{8}$$
$$= 0.68$$

Packing fraction is equal to 68% and hence BCC structure is not closely packed structure.

Tungsten, sodium, Iron and chromium have this type of structure.

⟨II⟩ Simple Cubic structure (SC)

The conventional unit cell of SC structure is the same as its primitive cell and is shown in below Fig.1.

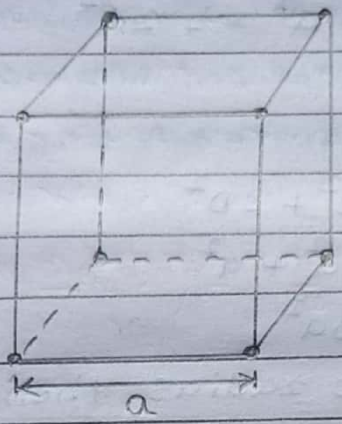


Fig.1 unit cell of SC structure

The atoms are located at the corners only and touch one another along the cube edges. Each atom has only six nearest neighbours. Hence the co-ordination number is six. Thus in the SC structure, we have

$$a = 2r$$

The number of atoms in a unit cell of simple cube

$$= 8 \times \frac{1}{8} = 1$$

$$\text{Packing fraction} = \frac{\text{Volume of all atoms in unit cell}}{\text{Volume of the unit cell}}$$

$$= \frac{1 \times 4/3 \pi r^3}{a^3} = \frac{4\pi r^3}{3(2r)^3} \quad (a = 2r$$

$$= \frac{4\pi r^3}{3 \times 8 \times r^3} = \frac{\pi}{6}$$

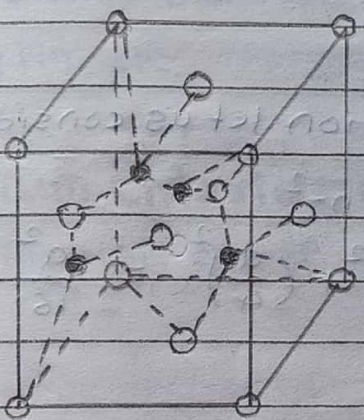
$$= 0.52$$

Thus the packing fraction is about 52%. Therefore this structure is a loosely packed at a given temperature.

Only polonium exhibit this type of structure.

* Structure of Diamond

Diamond exhibit both cubic and hexagonal type structures. The diamond cubic (DC) structure is more common structure. The space lattice of the diamond cubic structure is FCC with base consisting of two carbon atoms, one located at the lattice point and the other at a distance of one quarter of the body diagonal from the lattice point along the body diagonal. The unit cell of the diamond cubic structure is shown in Fig. 1



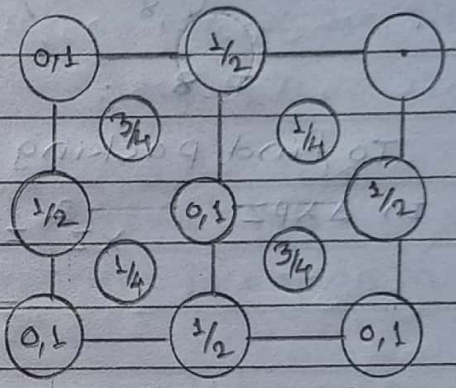


Fig 2 Plane view of DC structure

○ : C atom occupying FCC position

● : C atom occupying tetrahedral site

Fig 1 The unit cell of DC structure

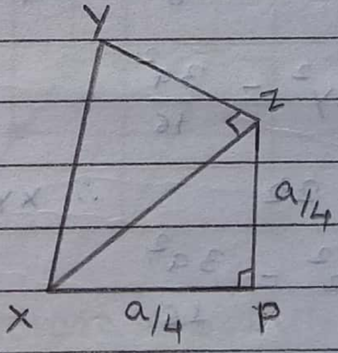


Fig. 3

The DC structure may also be viewed as an interpretation of two FCC sub-lattices with their origins at (0, 0, 0) and ($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$). A plane view of the positions of all the carbon atoms in the unit cell is shown in Fig. 2

Each atom of this structure has only four nearest neighbours i.e its co-ordination number is 4. In the unit cell, in ~~ad~~ addition to the eight corner atoms, there are six face centred atoms and four more atoms located inside the unit cell as shown in Fig. 2.

Each corner atom is shared by eight adjacent unit cells and each face centred atom is shared by two unit cells. Hence, the total number of atoms per unit cell

$$= \left(\frac{1}{8}\times 8\right) + \left(\frac{1}{2}\times 6\right) + 4 = 1+3+4$$

$$= 8$$

To find packing fraction let us consider Fig. 3.

In ΔXPZ, $$XZ^2 = XP^2 + PZ^2$$

$$= \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 = \frac{a^2}{16} + \frac{a^2}{16} = \frac{2a^2}{16}$$

$$XZ^2 = \frac{a^2}{8}$$

From ΔXYZ, $$XY^2 = XZ^2 + YZ^2$$

$$= \frac{a^2}{8} + \left(\frac{a}{4}\right)^2 = \frac{a^2}{8} + \frac{a^2}{16} = \frac{3a^2}{16}$$

$$XY^2 = \frac{3a^2}{16}$$

But $XY = 2r$ $\therefore XY^2 = 4r^2$

$$\therefore 4r^2 = \frac{3a^2}{16}$$

$$r^2 = \frac{3a^2}{4\times 16} = \frac{3a^2}{64}$$

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

$$\text{Packing fraction} = \frac{\text{volume of all atoms in unit cell}}{\text{volume of the unit cell}}$$

$$= \frac{8 \times \frac{4}{3}\pi r^3}{a^3} = \frac{8 \times \frac{4}{3}\pi \left(\frac{\sqrt{3}a}{8}\right)^3}{a^3}$$

$$= \frac{8 \times 4\pi (\sqrt{3})^3 a^3}{3a^3 \ (8)^3}$$

$$= \frac{8 \times 4\pi \ 3\sqrt{3}}{3 \times 8 \times 8 \times 8} = \frac{\sqrt{3}\pi}{16}$$

$$= 0.34 \text{ or } 34\%$$

So, it is loosely packed structure. other materials exhibiting this type of structure are Si, Ge, SiC, GaAs, gray tin, etc.

* Sodium Chloride (NaCl) structure

The unit cell of NaCl structure is shown in Fig. 1.

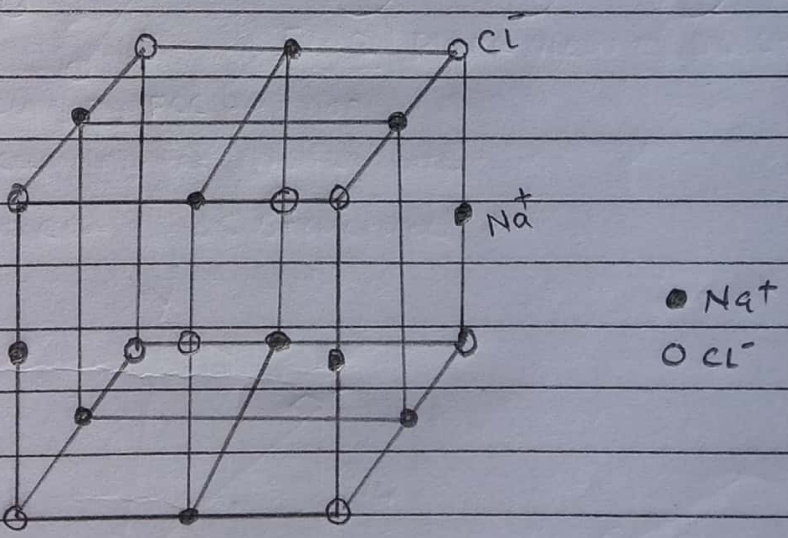


Fig 1 structure of sodium chloride

Sodium chloride structure is shown in above fig. sodium chloride ~~structure is~~ crystal is an ionic crystal. In the sodium lattice, the sodium ion and chloride ion are situated side by side. It consists of two FCC sub-lattices, one belonging to Na^+ ions with its origin at the point (0,0,0) and other belonging to Cl^- ions with its origin at the point $(a/2, 0, 0)$.

Each ion in the sodium chloride lattice has six nearest neighbour ions at a distance $a/2$. Its co-ordination number is 6.

The ionic radius of Chlorine = 1.81 Å

The ionic radius of sodium = 0.98 Å

Each unit cell in sodium chloride has four sodium ions and four associated chlorine ions. Thus, there are 4 molecules in each unit cell.

The positions of various ions in the unit cell are as follows:

Na^+ : $0,0,0;\ \frac{1}{2},\frac{1}{2},0;\ \frac{1}{2},0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2}$

Cl^- : $\frac{1}{2},\frac{1}{2},\frac{1}{2};\ 0,0,\frac{1}{2};\ 0,\frac{1}{2},0;\ \frac{1}{2},0,0$