Module-I

Crystal Structures

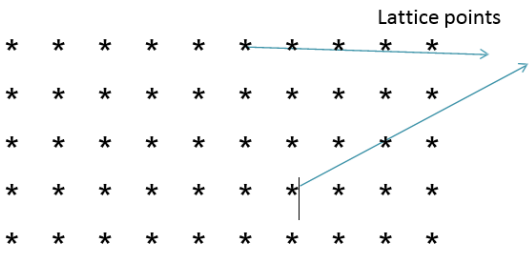
PART-B Long Answer Questions

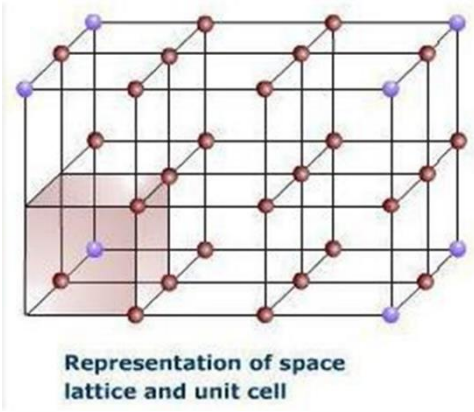
1. Explain the concepts space lattice, basis, unit cell and lattice parameter.

Ans.

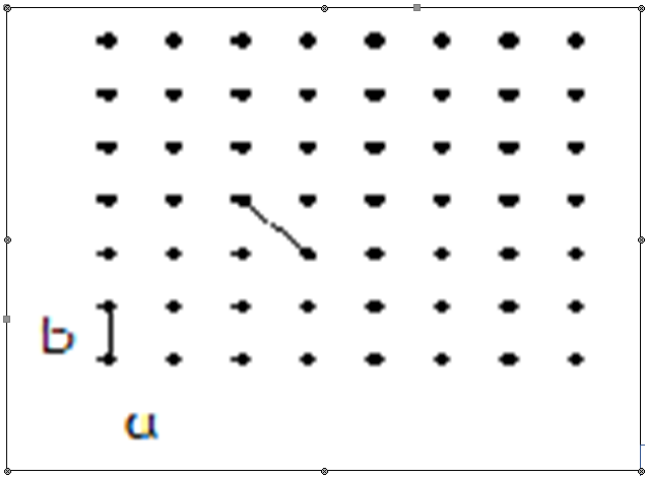
Space Lattice (or) Crystal Lattice:

The regular orderly arrangement of lattice points in space which resembles the atoms or molecules in a crystal such that every point has same environment with respect to all other points is known as space lattice (or) crystal lattice.




Representation of space lattice and unit cell

- A space lattice is defined as an infinity array of points in three dimensions in which every point has identical surroundings to that of every other point.
- Consider a two dimensional array of lattice points as shown in figure.



- By repeated translation of vectors a, b on the plane of the paper, we can generate the square array.
- The magnitude of a and b are equal and can be taken to be unity. The angle between a and b is 90°, a and b are called fundamental translational vectors that generate square array.
- Let n_1 be the number of translations of magnitude a in x-direction then its translation vector $\overrightarrow{T_1} = n_1\vec{a}$
- Let n_2 be the number of translations of magnitude b in y-direction then its translation vector $\overrightarrow{T_2} = n_2\vec{b}$

Let $\underset{T}{\rightarrow}$ be the resultant translation vector.

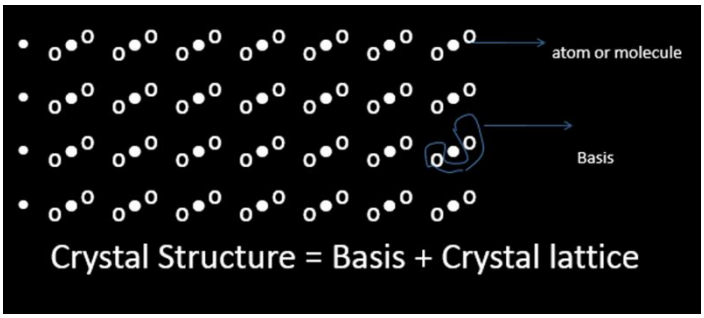
So, $\underset{T}{\rightarrow} = \underset{T_1}{\rightarrow} + \underset{T_2}{\rightarrow}$

$\underset{T}{\rightarrow} = n_1 \underset{a}{\rightarrow} + n_2 \underset{b}{\rightarrow}$ where n_1 and n_2 are integers.

In 3-D $\underset{T}{\rightarrow} = n_1 \underset{a}{\rightarrow} + n_2 \underset{b}{\rightarrow} + n_3 \underset{c}{\rightarrow}$

Basis:

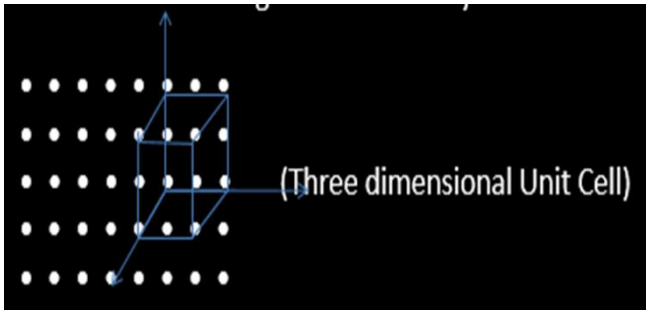
The set of atoms or molecules attached to each lattice point in a crystal structure, identical in composition, arrangement and orientation, is called the basis of a crystal lattice.

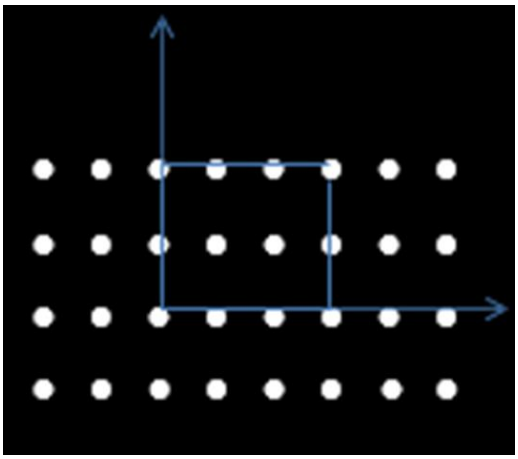


Unit Cell:

- An unit cell is the smallest geometric figure, the repetition of which in three dimensions will give the actual crystal structure.
- Hence, the unit cell may be now defines as 'the smallest fundamental elementary pattern of minimum of atoms (molecules or group of molecules) which represents fully all the characteristics of the crystal'.
- The choice of a unit cell may be of different types as shown in fig.
- In two dimensions a unit cell is called as a parallelogram whereas in three dimensions it is called as parallelepiped.

Two dimensional unit cell

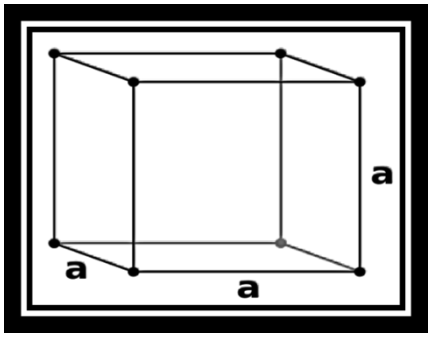


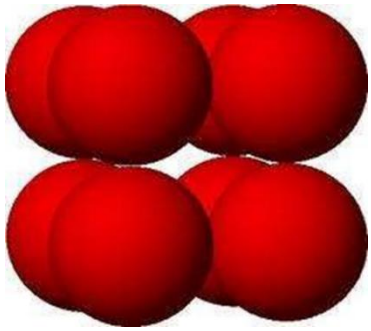


Types of Unit cell:

Primitive cell (P):

- Parallelepiped, formed by lattice points only at their corners are called as primitive cell or simple cell.
- The primitive cell is defined as “a unit cell which contains lattice points at corners only’.
- Such cell contains effectively one lattice point per cell, i.e., one lattice point as associated with each primitive cell.
- Example for primitive cell: Simple Cubic unit cell.





Non primitive cell or Multiple Cell:

- If a unit cell contains more than one lattice point then it is called as a multiple cell or non primitive cell.

  Examples for non-primitive cell: BCC and FCC unit cell.

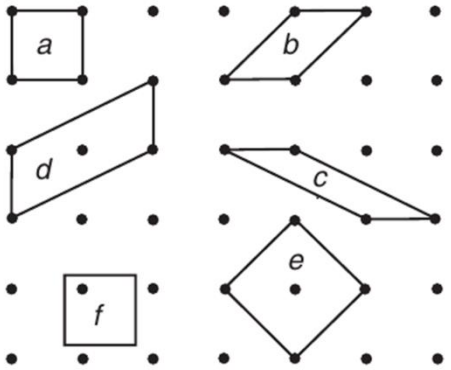


Fig: Primitive and non-primitive unit cells in 2-dimsensions.

Lattice Parameters

Crystallographic Axes: These are the lines drawn parallel to the lines of intersection of any three faces of the unit cell which do not lie in the same plane. ox,oy,oz

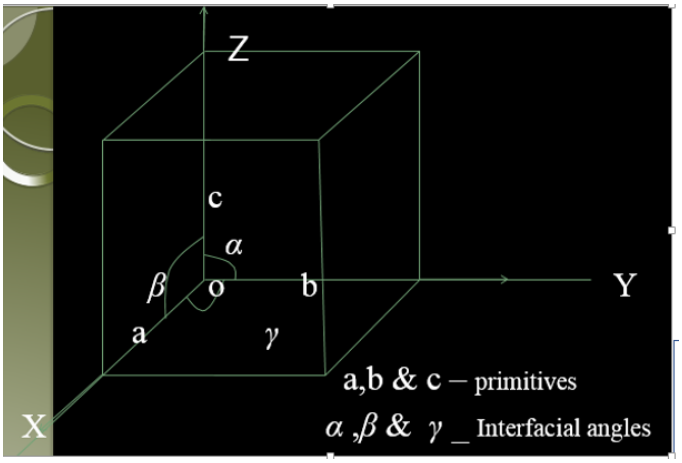
Primitives: The three sides of unit cell are called Primitives. They are denoted by a,b,c. They are also known as lattice constants.

Interfacial angles: The angles between three crystallographic axes of the unit cell are called interfacial angles.

The angle b/w Y and Z axis is α

Z and X axes is β X and

Y axes is γ



2. Enlist the seven crystal systems, draw their diagrams neatly.

Crystal Systems:

There are 32 classes of crystals based on geometrical considerations. Taking different symmetries and structures into consideration, all these structures are classified into seven crystal systems. Each system is characterized by the values of a,b,c and α, β, γ.

The seven crystal systems are given as

1.Cubic

2.Tetragonal

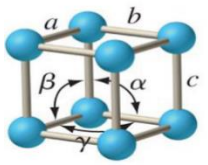
3. Orthorhombic

4. Trigonal (or) Rhombohedral

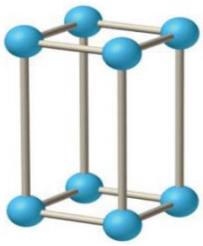
5. Monoclinic

6.Triclinic

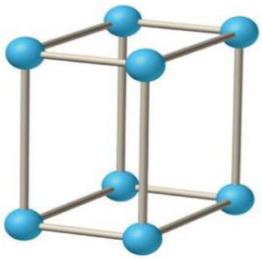
7. Hexagonal



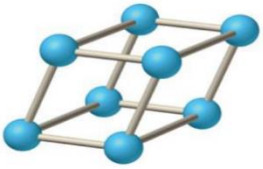
Simple cubic
$a = b = c$
$\alpha = \beta = \gamma = 90^\circ$



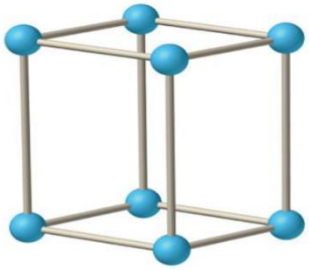
Tetragonal
$a = b \neq c$
$\alpha = \beta = \gamma = 90^\circ$



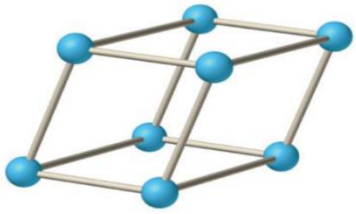
Orthorhombic
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90^\circ$



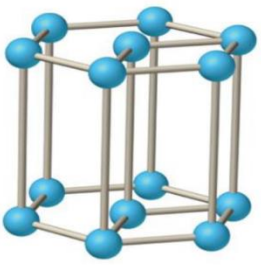
Rhombohedral (or) Trigonal
$a = b = c$
$\alpha = \beta = \gamma \neq 90^\circ$



Monoclinic
$a \neq b \neq c$
$\gamma \neq \alpha = \beta = 90^\circ$



Triclinic
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90^\circ$



Hexagonal
$a = b \neq c$
$\alpha = \beta = 90^\circ, \gamma = 120^\circ$

Seven Crystal Systems and its Lattice Parameters

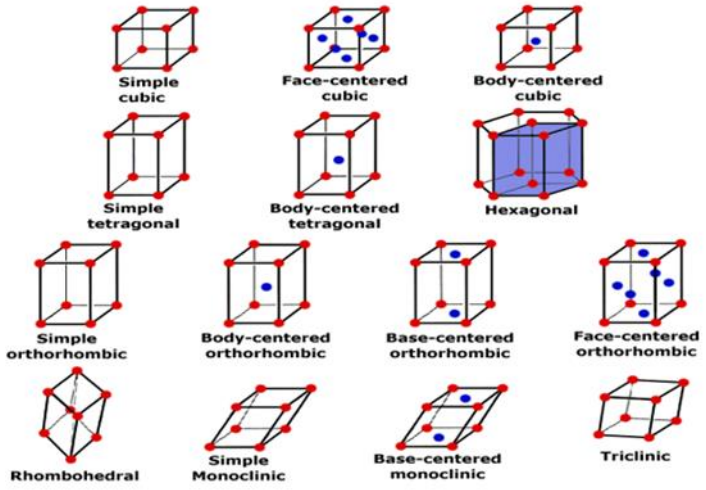
Sno	System	Unit cell characteristics	Bravais lattices	No. of lattices in the system
1	CUBIC	a=b=c; α=β=γ=90⁰	P, I, F	3
2	TETRAGONAL	a=b≠c; α=β=γ=90⁰	P, I	2
3	ORTHORHOMBIC	a≠b≠c; α=β=γ=90⁰	P, C, I, F	4
4	TRIGONAL	a=b=c; α=β=γ≠90⁰< 120	P	1
5	MONOCLINIC	a≠b≠c; α=γ=90⁰≠β	P, C	2
6	TRICLINIC	a≠b≠c; α≠β≠γ	P	1
7	HEXAGONAL	a=b≠c;α=β=90⁰;γ=120⁰	P	1

3. Draw the fourteen Bravais lattices.

Bravais lattices:

- A three dimensional space lattice is generated by repeated translation of three non-coplanar vectors a, b and c.
- In 1948 Bravais showed that, there are fourteen ways of arranging points in space lattice, under the seven crystal systems to describe crystals.
- The different Bravais lattices and their crystal systems are listed in given table.
- 3 Dimensions : Fourteen Bravais Lattices Only 14 ways of arranging the points in space 14 Space Lattices - Bravais Lattices Belong to Seven Crystal Systems.

4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred (Base-Centered)
+
7 Crystal Classes
→ 14 Bravais Lattices



4. Define co-ordination number, packing fraction and obtain the packing fraction of SC

Ans.

Co-ordination number:

- Co-ordination number is the number of nearest neighbouring atoms to a particular atom. (or) Co-ordination number is the number of nearest neighbours directly surrounding a given atom.
- More closely packed structures have greater co-ordination number.
- Simply, co-ordination number of an atom is the number of atoms which it touches.
- The co-ordination number of Sc, BCC, FCC are 6, 8, 12 respectively.

Packing Factor or Packing Fraction or Atomic Packing Factor

It is also called Packing density.

Atomic packing factor is the ratio of volume occupied by atoms in a unit cell to the total volume of the unit cell.

$$APF = \frac{Zv}{V} = \frac{Z_{atom} v_{atom}}{V_{atom}} \qquad (1)$$

Packing factor is dimension less and is always less than unity.

Where, z = Total number of atoms per unit cell

v = volume of one atom

V = Total volume of the unit cell

Packing fraction of SC

Volume of one atom (spherical) is $= \frac{4}{3}\pi r^3$ (2)

We know that, the radius of atom in simple cubic is

$$r = a/2 \qquad (3)$$

Volume of the unit cell (V) = length x breadth x height

We know that for a cubic system, Length = breath = height = a

V = a x a x a

$V = a3$ ……. (6)

Substitute equation (5) and (6) in equation (1) we get, atomic packing factor (APF) is,

$APF = \frac{\pi a^3/6}{a^3}$

APF = π/6

or APF = 0.52 …… (7)

Therefore, we can say that 52% volume of the unit cell of SC is occupied by atoms and remaining 48% volume is vacant. Thus, the packing density is 52%. Since the packing density is very low, SC has loosely packed structure.

5. Define atomic packing fraction and obtain the packing fraction of BCC

Atomic packing factor

Atomic packing factor is the ratio of volume occupied by atoms in a unit cell to the total volume of the unit cell.

$$APF = \frac{Zv}{V} = \frac{Z_{atom} v_{atom}}{V_{atom}} \qquad (1)$$

Packing factor is dimension less and is always less than unity.

Where, z = Total number of atoms per unit cell

v = volume of one atom

V = Total volume of the unit cell

Packing fraction of BCC

$$APF = zv/V \qquad \ldots\ldots\ldots\ldots (1)$$

In body-centred cubic structure,

The number of atoms per unit cell = 2

Volume of an atom (spherical) is = $4/3\ \pi r^3$…… (2)

We know that, the atomic radius of BCC is r =$(a\sqrt{3})/4$…….. (3)

Volume occupied by the total number of atoms per unit cell is

$$zv = 2 \times 4/3\ \pi r^3 \ldots\ldots\ldots\ldots\ldots (4)$$

Substitute equation (3) in (4) we get,

$$zv = \frac{8\pi}{3}\left[\frac{a\sqrt{3}}{4}\right]^3$$

$$zv = \pi a^3 \frac{\sqrt{3}}{8} \ldots\ldots\ldots\ldots\ldots\ldots (5)$$

Volume of the unit cell for a cubic system is

$V = a^3$ …….. (6)

Substitute equation (5) and (6) in equation (1) we get,

Atomic pacing factor (APF) = $\frac{\pi a^3 \frac{\sqrt{3}}{8}}{a^3}$

APF = $\frac{\pi\sqrt{3}}{8}$

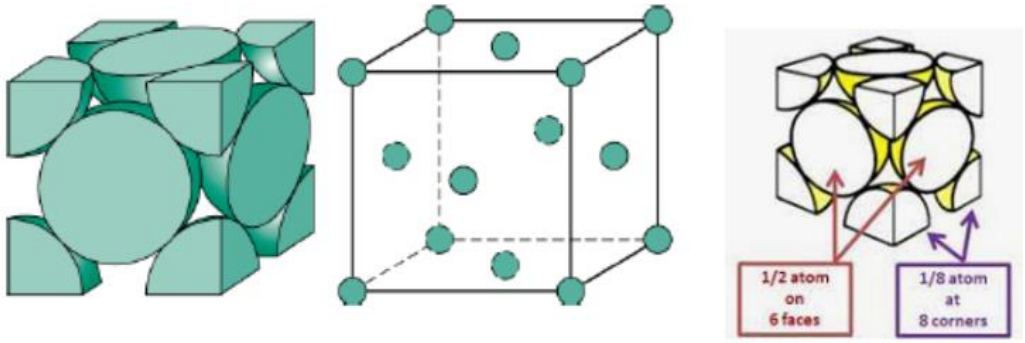
APF = 0.68 …….. (7)

Therefore, we can say that 68% volume of the unit cell of BCC is occupied by atoms and remaining 32% volume is vacant.

6. Explain the FCC structure and obtain the packing fraction of FCC

Face Centred Cubic Structure (FCC)

A face centred cubic (FCC) structure unit cell consists of eight corner atoms and six face centred atoms. A face centred cubic unit cell is shown in given figure.



Packing fraction of FCC

APF = $\frac{zv}{V}$ ……..(1)

In face-centred cubic structure,

The number atoms per unit cell = 4

Volume of atoms is = $\frac{4}{3}\pi r^3$ ……..……. (2)

We know that, the atomic radius of FCC is

r = $\frac{a\sqrt{2}}{4}$ ……..…….. (3)

Volume occupied by the atoms per unit cell is

$zv = 4 \times \frac{4}{3}\pi r3$ ..... (4)

Substitute equation (3) in (4) we get,

$$zv = \frac{16\pi}{3}\left[\frac{a\sqrt{2}}{4}\right]^3$$

$$zv = \frac{16\pi}{3}\left[\frac{a\sqrt{2}}{4}\right]^3$$

$$zv = \pi a^3 \frac{\sqrt{2}}{6} \text{.....(5)}$$

Volume of the unit cell for a cubic system is

$V = a^3$ ..... (6)

Substitute equation (5) and (6) in equation (1) we get,

Atomic packing factor (APF) = $\frac{\frac{\pi a^3\sqrt{2}}{6}}{a^3}$

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

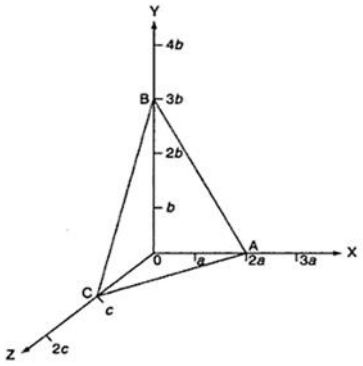
APF =0.74 ..... (7)

Therefore, we can say that 74% volume of the unit cell of FCC is occupied by atoms and remaining 26% volume is vacant.

7. What are miller indices? Explain the rules for defining miller indices with an example. Show the planes (100), (110) and (111).

MILLER INDICES

- Miller Indices are three numbers used to label lattice planes.
- Miller Indices were introduced in 1839 by the British mineralogist William Hallowes Miller.
- The Miller index gives a mathematical description to explain lattice directions and lattice planes.
- The Miller Indices are the three smallest possible integers which have the same ratios as the reciprocals of the intercepts of the plane concerned on the three axes.



The rules for finding Miller Indices are:

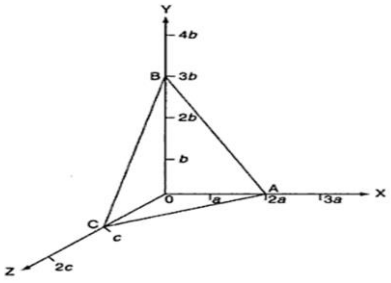
- Choose a system of three co-ordinate axes along the crystallographic axes.
- First find the intercepts of plane on three axes in terms of primitives.
- Let the intercepts are pa, qb, rc where a, b, c are primitives and p, q, r are integers or fractions.
- Take the reciprocals of p, q, r
- i.e., Now Miller Indices h, k, l such that
- h: k: l = 1/p: 1/q: 1/r

- The below figure shows a plane making intercepts 2a, 3b, c along X, Y, Z directions.
- The intercepts in multiples of lattice parameters are 2, 3, 1
- The reciprocals of intercepts are $\frac{1}{2}, \frac{1}{3}, \frac{1}{1}$

- Clear these fractions [by multiplying with LCM] to smallest integers having the same ratio as the fractions, enclose these integers in brackets.

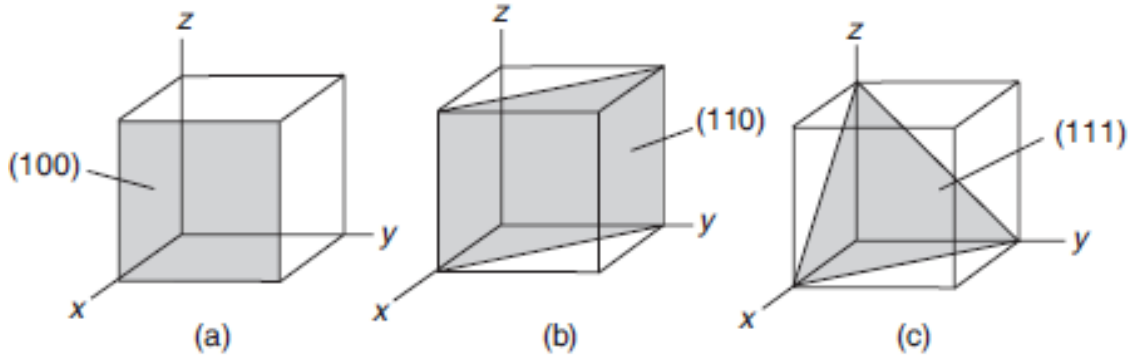
$$\frac{1}{2} \times 6, \frac{1}{3} \times 6, \frac{1}{1} \times 6$$
$$3 \quad 2 \quad 6$$

- So the miller indices are (3, 2, 6)



Procedure for finding Miller Indices

- Step 1 : Determine the intercepts of the plane along the axes
- Step 2 : Determine the reciprocals of these numbers.
- Step 3 : Find the LCM and multiply each by this LCM
- Step 4 : Write it in paranthesis in the form (h k l).



8. Obtain the equation for interplanar spacing for orthogonal systems. Calculate the ratio of the planes (100), (110) and (111).

Interplanar Spacing

- The distance 'd' between successive lattice planes is known as the inter-planar distance.
- The inter-planar distance 'd' involves the axial lengths of the unit cell and the Miller indices of the planes. We shall derive here an expression for d in the case of a cubic system only.
- We know that the three axes of a cubic crystal are mutually perpendicular.
- Let ABC be one of the family of parallel lattice planes in the crystal (Fig).

Let its Miller indices be (hkl) and the intercepts on the crystallographic axes be,

OA = a/h , OB = b/k , and OC = c/l.

The next plane of the set parallel to ABC passes through the origin of the coordinates O (which is not shown in the Fig.).

Therefore, ON, the length of the normal from the origin to the plane is equal to 'd'.

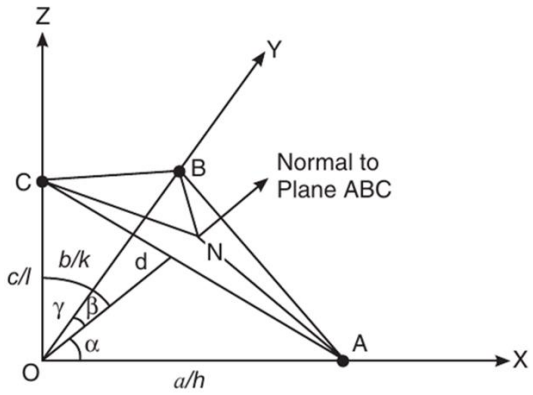


Fig. Determination of interplanar distance in a cubic crystal

Let α, β, and γ be the angles ON makes with the three crystallographic axes respectively.

Then the direction cosines of ON are

$$\cos\alpha = \frac{ON}{OA} = \frac{d}{a/h}$$

$$\cos\beta = \frac{ON}{OB} = \frac{d}{b/k}$$

$$\cos\gamma = \frac{ON}{OC} = \frac{d}{c/l}$$

The sum of the squares of the direction cosines of a line equals unity. Thus,

$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$$

Substituting the values of cosα, cosβ, cosγ, in the above equation,

$$\frac{d^2}{a^2/h^2}+\frac{d^2}{b^2/k^2}+\frac{d^2}{c^2/l^2}=1$$

$$d^2\left[\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}\right]=1$$

$$d=\left[\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}\right]^{-1/2}$$

In case of cubic system, a=b=c. So,

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

Lattice Planes are (100), (110), (111) We have,

$$d_{(100)}=\frac{a}{\sqrt{1^2+0+0}}=a$$

$$d_{(110)}=\frac{a}{\sqrt{1^2+1^2+0}}=\frac{a}{\sqrt{2}}$$

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

Thus $d_{(100)} : d_{(110)} : d_{(111)} = 1 : 1/\sqrt{2} : 1/\sqrt{3}$

$= 1 : 0.707 : 0.577$

9. Write a short note on lattice parameter, derive an expression for lattice parameter based on density of the atom, volume of the unit cell.

Lattice Parameters

Crystallographic Axes: These are the lines drawn parallel to the lines of intersection of any three faces of the unit cell which do not lie in the same plane. ox,oy,oz

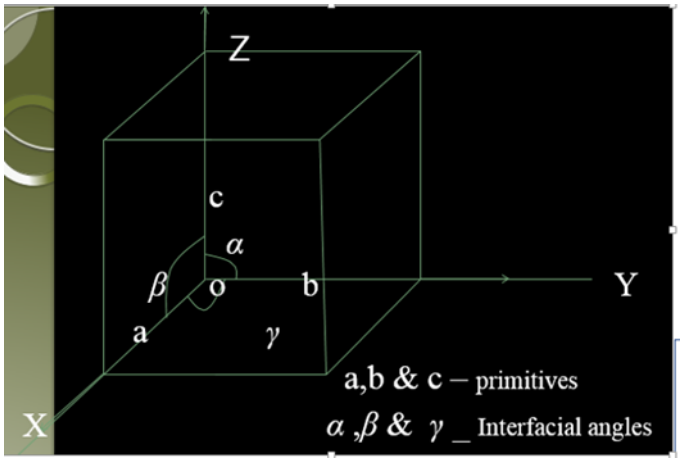
Primitives: The three sides of unit cell are called Primitives. They are denoted by a,b,c. They are also known as lattice constants.

Interfacial angles: The angles between three crystallographic axes of the unit cell are called interfacial angles.

The angle b/w Y and Z axis is α

Z and X axes is β X and

Y axes is γ



Expression for Lattice Constant

In a cubic unit cell, the sides of the cube are equal and constant, which is known as lattice constant.

a = b = c = lattice constant (a)

Consider a cubic unit cell with lattice parameters a = b = c and

$\alpha = \beta = \gamma = 90^o$

Let ρ be the density of the cell

Mass of the cubic unit cell $= a^3\rho$ ….(1)

If M is the molecular weight of the cell and NA is the Avogadro's number,

Mass of each atom in unit cell = M / N_A

If n is number of atoms in a unit cell, then

Mass of the cubic unit cell = nM / N_A …(2)

from (1) and (2), $a^3\rho = nM / N_A$

$a^3 = nM / \rho N_A$

$a = [nM / \rho N_A]^{1/3}$

10. Define the packing density, Obtain the packing fractions of SC, BCC, FCC

Packing density or Packing Fraction or Atomic Packing Factor

Atomic packing factor is the ratio of volume occupied by atoms in a unit cell to the total volume of the unit cell.

$$APF = APF = \frac{Zv}{V} = \frac{Z_{atom}v_{atom}}{V_{atom}} \quad (1)$$

Packing factor is dimension less and is always less than unity.

Where, z = Total number of atoms per unit cell

v = volume of one atom

V = Total volume of the unit cell

Packing fraction of SC

Volume of one atom (spherical) is = $\frac{4}{3}\pi r^3$ (2)

We know that, the radius of atom in simple cubic is

$$r = a/2 \quad (3)$$

Volume of the unit cell (V) = length x breadth x height

We know that for a cubic system, Length = breath = height = a

V = a x a x a

$V = a^3$ ……. (6)

Substitute equation (5) and (6) in equation (1) we get, atomic packing factor (APF) is,

$APF = \frac{\pi a^3/6}{a^3}$

APF = $\pi/6$ …… (7)

Therefore, we can say that 52% volume of the unit cell of SC is occupied by atoms and remaining 48% volume is vacant. Thus, the packing density is 52%. Since the packing density is very low, SC has loosely packed structure.

Packing fraction of BCC

APF = zv/V ……. (1)

In body-centred cubic structure,

The number of atoms per unit cell = 2

Volume of an atom (spherical) is = 4/3 πr^3…… (2)

We know that, the atomic radius of BCC is r =($a\sqrt{3}$)/4…….. (3)

Volume occupied by the total number of atoms per unit cell is

zv = 2 × 4/3 πr^3 …….. (4)

Substitute equation (3) in (4) we get,

$$zv = \frac{8\pi}{3}\left[\frac{a\sqrt{3}}{4}\right]^3$$

$$zv = \pi a^3 \frac{\sqrt{3}}{8} \text{ …….(5)}$$

Volume of the unit cell for a cubic system is

$V = a^3$ …….. (6)

Substitute equation (5) and (6) in equation (1) we get,

Atomic pacing factor (APF) = $\frac{\pi a^3 \frac{\sqrt{3}}{8}}{a^3}$

$$APF = \frac{\pi\sqrt{3}}{8}$$

APF = 0.68 …….. (7)

Therefore, we can say that 68% volume of the unit cell of BCC is occupied by atoms and remaining 32% volume is vacant.

Packing fraction of FCC

APF = $\frac{zv}{V}$ ……..(1)

In face-centred cubic structure,

The number atoms per unit cell = 4

Volume of atoms is = $\frac{4}{3}\pi r^3$ …….…… (2)

We know that, the atomic radius of FCC is

$r = \frac{a\sqrt{2}}{4}$ ……..…….. (3)

Volume occupied by the atoms per unit cell is

$zv = 4 \times \frac{4}{3}\pi r3$ …… (4)

Substitute equation (3) in (4) we get,

$$zv = \frac{16\pi}{3}\left[\frac{a\sqrt{2}}{4}\right]^3$$

$$zv = \frac{16\pi}{3}\left[\frac{a\sqrt{2}}{4}\right]^3$$

$$zv = \pi a^3 \frac{\sqrt{2}}{6} \text{.....(5)}$$

Volume of the unit cell for a cubic system is

$V = a^3$ …… (6)

Substitute equation (5) and (6) in equation (1) we get,

Atomic packing factor (APF) = $\frac{\frac{\pi a^3\sqrt{2}}{6}}{a^3}$

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

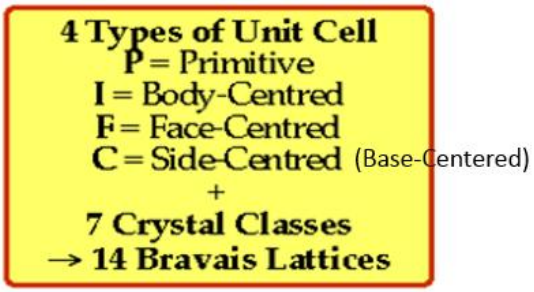
APF =0.74 …… (7)

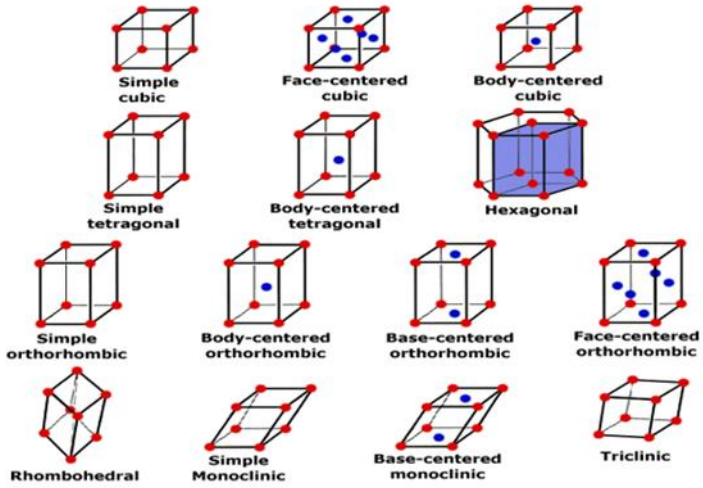
Therefore, we can say that 74% volume of the unit cell of FCC is occupied by atoms and remaining 26% volume is vacant.

11.What are Bravais lattices? Draw the Bravais lattices for Orthogonal systems.

- A three dimensional space lattice is generated by repeated translation of three non-coplanar vectors a, b and c.
- In 1948 Bravais showed that, there are fourteen ways of arranging points in space lattice, under the seven crystal systems to describe crystals.

- The different Bravais lattices and their crystal systems are listed in given table.
- 3 Dimensions : Fourteen Bravais Lattices Only 14 ways of arranging the points in space 14 Space Lattices - Bravais Lattices Belong to Seven Crystal Systems.





12. Explain the seven crystal systems based on interfacial angles and interatomic distances and mention the Bravais lattice strutures for each crystal system.

Ans. Write 2 & 3 Question answers

13. List the type of lattice arrangements in crystals. Explain them with neat diagrams.

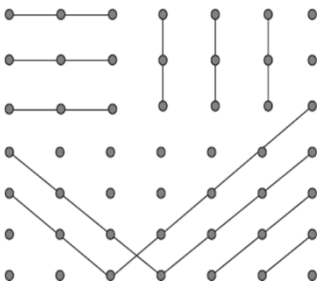
Ans. Write 2 Question answer

14. Prove that the FCC has the highest packing fraction than SC and BCC.

Ans. Write 10th Question Answer

15. What are lattice planes? Obtain the interplanar seperation of simple cubic lattice.

Ans. Lattice planes:



- The crystal lattice may be regarded as made up of aggregate of a set of parallel equidistant planes passing through the lattice points are known as lattice planes.
- The lattice planes can be chosen in many ways as like in figure.
- Lattice planes are generally parallel and equally spaced planes.
- Generally, the lattice planes are characterised by miller indices and interplanar distance i.e., (h, k, l) and ‘d’ respectively.
- Each family of lattice planes have an interplanar spacing ‘d’.

- # Interplanar Spacing

Write 8th Question Answer

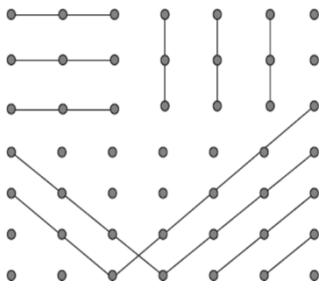
16. Differentiate SC, BCC and FCC strutures based on coordination number, nearest neighbour distance, atomic radius and atomic paking fraction.

Ans.

Sr.No.	Characteristics	Unit Cell		
		SC	BCC	FCC
1.	Unit cell volume, V	a^3	a^3	a^3
2.	Atoms per unit cell, Z	1	2	4
3.	Atomic radius, r	$a/2$	$a\sqrt{3}/4$	$a/2\sqrt{2}$
4.	Coordination number, CN	6	8	12
5.	Atomic packing fraction, APF	$\pi/6$ $= 0.52$	$\pi\sqrt{3}/8$ $= 0.68$	$\pi/3\sqrt{2}$ $= 0.74$
6.	Void space	48%	32%	26%
7.	Density, ρ	$\frac{M}{N_A a^3}$	$\frac{2M}{N_A a^3}$	$\frac{4M}{N_A a^3}$

17. What are lattice planes? Explain the concept of miller indices, Obtain miller indices for a plane making intercepts pa,qb,rc with crsytallographic axes

Ans. Lattice planes:



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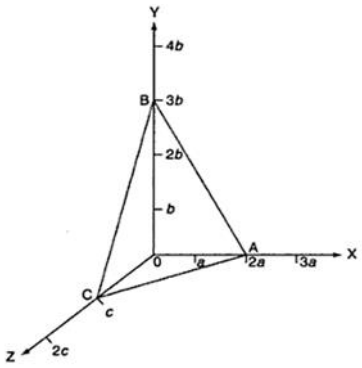
- The lattice planes can be chosen in many ways as like in figure.
- Lattice planes are generally parallel and equally spaced planes.
- Generally, the lattice planes are characterised by miller indices and interplanar distance i.e., (h, k, l) and ‘d’ respectively.
- Each family of lattice planes have an interplanar spacing ‘d’.

MILLER INDICES

- Miller Indices are three numbers used to label lattice planes.
- Miller Indices were introduced in 1839 by the British mineralogist William Hallowes Miller.

- The Miller index gives a mathematical description to explain lattice directions and lattice planes.
- The Miller Indices are the three smallest possible integers which have the same ratios as the reciprocals of the intercepts of the plane concerned on the three axes.



The rules for finding Miller Indices are:

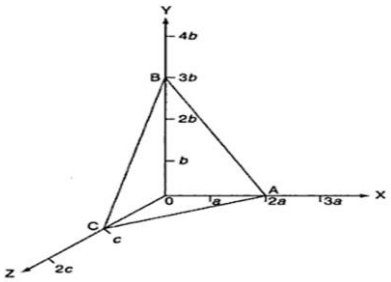
- Choose a system of three co-ordinate axes along the crystallographic axes.
- First find the intercepts of plane on three axes in terms of primitives.
- Let the intercepts are pa, qb, rc where a, b, c are primitives and p, q, r are integers or fractions.
- Take the reciprocals of p, q, r
- i.e., Now Miller Indices h, k, l such that
- h: k: l = 1/p: 1/q: 1/r

- The below figure shows a plane making intercepts 2a, 3b, c along X, Y, Z directions.
- The intercepts in multiples of lattice parameters are 2, 3, 1
- The reciprocals of intercepts are $\frac{1}{2}, \frac{1}{3}, \frac{1}{1}$

- Clear these fractions [by multiplying with LCM] to smallest integers having the same ratio as the fractions, enclose these integers in brackets.

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

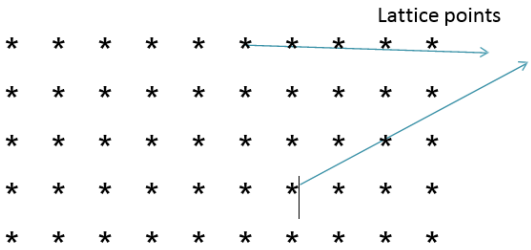
- So the miller indices are (3, 2, 6)

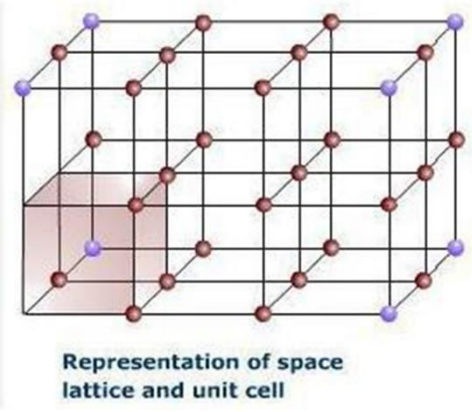


18. Define space lattice and explain the concept of space lattice for a 2-D array of infitesimal points, also explain the concept of basis and relate them

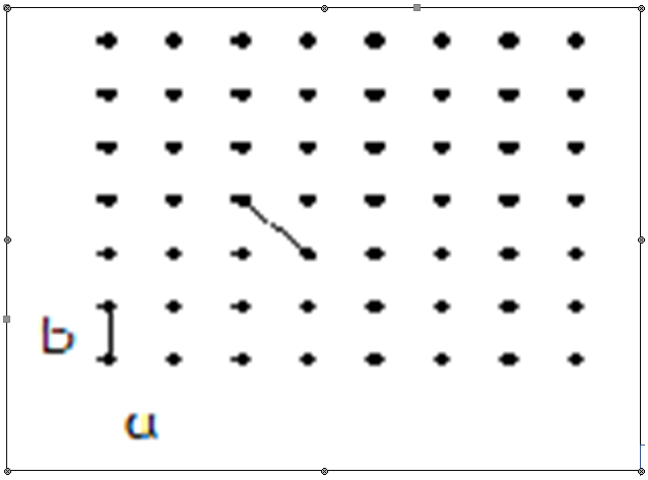
Ans. Space Lattice (or) Crystal Lattice:

The regular orderly arrangement of lattice points in space which resembles the atoms or molecules in a crystal such that every point has same environment with respect to all other points is known as space lattice (or) crystal lattice.





- A space lattice is defined as an infinity array of points in three dimensions in which every point has identical surroundings to that of every other point.
- Consider a two dimensional array of lattice points as shown in figure.



- By repeated translation of vectors a, b on the plane of the paper, we can generate the square array.
- The magnitude of a and b are equal and can be taken to be unity. The angle between a and b is 90°, a and b are called fundamental translational vectors that generate square array.
- Let n_1 be the number of translations of magnitude a in x-direction then its translation vector $\overrightarrow{T_1} = n_1\vec{a}$
- Let n_2 be the number of translations of magnitude b in y-direction then its translation vector $\overrightarrow{T_2} = n_2\vec{b}$

Let $\underset{T}{\rightarrow}$ be the resultant translation vector.

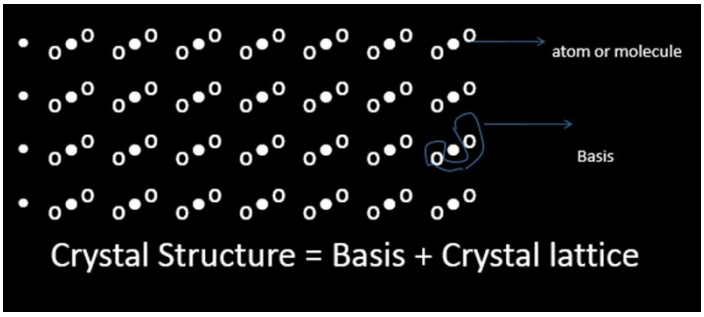
So, $\underset{T}{\rightarrow} = \underset{T_1}{\rightarrow} + \underset{T_2}{\rightarrow}$

$\vec{T} = n_1 \vec{a} + n_2 \vec{b}$ where n_1 and n_2 are integers.

In 3-D $\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$

Basis:

The set of atoms or molecules attached to each lattice point in a crystal structure, identical in composition, arrangement and orientation, is called the basis of a crystal lattice.



19. Explain the terms coordination number, nearest neighbour distance, atomic radius, packing fraction

Ans. Co-ordination number:

- Co-ordination number is the number of nearest neighbouring atoms to a particular atom. (or) Co-ordination number is the number of nearest neighbours directly surrounding a given atom.
- More closely packed structures have greater co-ordination number.
- Simply, co-ordination number of an atom is the number of atoms which it touches.
- The co-ordination number of Sc, BCC, FCC are 6, 8, 12 respectively.

Nearest neighbour distance

- The distance between the centers of two nearest neighbour atoms is called nearest neighbour distance.
- For Sc, BCC, FCC the nearest neighbor distance is a, $\sqrt{3}a/2$, $a/\sqrt{2}$ respectively.

Atomic radius

- ✓ The atomic radius 'r' is defined as half distance between nearest neighbour atoms in the unit cell.
- ✓ Atomic radius for Sc, BCC, FCC is a/2, $\sqrt{3}a/4$, $a/2\sqrt{2}$ respectively.

Packing Factor or Packing Fraction or Atomic Packing Factor

- ✓ It is also called Packing density.
- ✓ Atomic packing factor is the ratio of volume occupied by atoms in a unit cell to the total volume of the unit cell.

$$\text{APF} = \frac{zv}{V} = \frac{z_{atom} v_{atom}}{V_{unit\ cell}}$$

- ✓ Packing factor is dimension less and is always less than unity.

The packing fraction of Sc, BCC, FCC are 0.52, 0.68, 0.74 respectively.

20. Define atomic radius and nearest neighbour distance and obtain the relation between atomic radius and interatomic separation for SC, BCC and FCC

Ans. Atomic radius

- ✓ The atomic radius 'r' is defined as half distance between nearest neighbour atoms in the unit cell.
- ✓ Atomic radius for Sc, BCC, FCC is a/2, $\sqrt{3}$a/4, a/2$\sqrt{2}$ respectively.

Nearest neighbour distance

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Sr.No.	Characteristics	Unit Cell		
		SC	BCC	FCC
1.	Unit cell volume, V	a^3	a^3	a^3
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6.	Void space	48%	32%	26%
7.	Density, ρ	$\frac{M}{N_A a^3}$	$\frac{2M}{N_A a^3}$	$\frac{4M}{N_A a^3}$

PART-C Short Answer Questions

1. Explain the concept of space lattice

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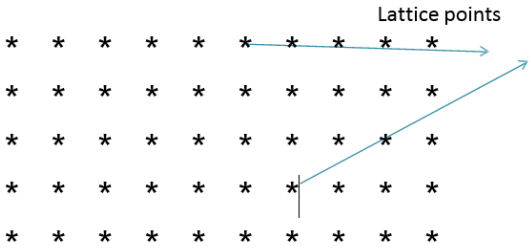
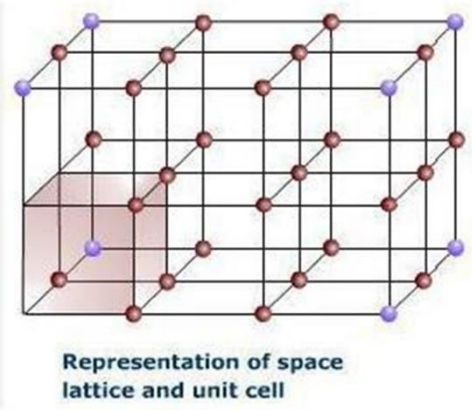


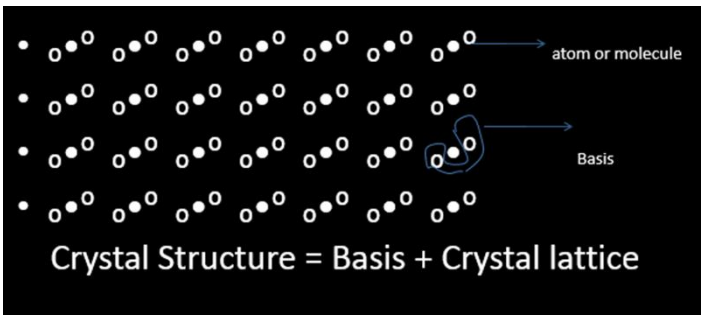


Representation of space lattice and unit cell

2. Explain the concept of basis

Ans. Basis:

The set of atoms or molecules attached to each lattice point in a crystal structure, identical in composition, arrangement and orientation, is called the basis of a crystal lattice.



3. How can we relate space lattice and basis to crystal structure

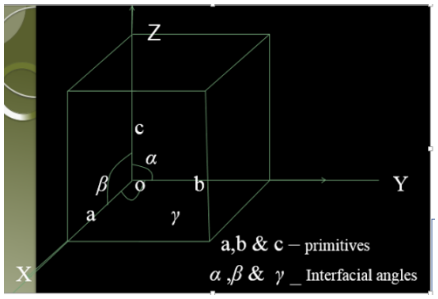
Ans. Write 1st and 2nd Questions Answers (short)

4. Obtain an equation for lattice parameter for a cubic system

Ans.

Expression for Lattice Constant

In a cubic unit cell, the sides of the cube are equal and constant, which is known as lattice constant.



a = b = c = lattice constant (a)

Consider a cubic unit cell with lattice parameters a = b = c and

$\alpha = \beta = \gamma = 90^o$

Let ρ be the density of the cell

Mass of the cubic unit cell $= a^3\rho$ ….(1)

If M is the molecular weight of the cell and NA is the Avogadro's number,

Mass of each atom in unit cell = M / N_A

If n is number of atoms in a unit cell, then

Mass of the cubic unit cell = nM / N_A …(2)

from (1) and (2), $a^3\rho = nM / N_A$

$a^3 = nM / \rho N_A$

$a = [nM / \rho N_A]^{1/3}$

5. List the seven crystal systems and mention relation interfacial angles and interatomic distances.

The seven crystal systems are given as

1.Cubic

2.Tetragonal

3. Orthorhombic

4. Trigonal (or) Rhombohedral

5. Monoclinic

6.Triclinic

7. Hexagonal

Sno	System	Unit cell characteristics	Bravais lattices	No. of lattices in the system
1	CUBIC	a=b=c; α=β=γ=90⁰	P, I, F	3
2	TETRAGONAL	a=b≠c; α=β=γ=90⁰	P, I	2
3	ORTHORHOMBIC	a≠b≠c; α=β=γ=90⁰	P, C, I, F	4
4	TRIGONAL	a=b=c; α=β=γ≠90⁰< 120	P	1
5	MONOCLINIC	a≠b≠c; α=γ=90⁰≠β	P, C	2
6	TRICLINIC	a≠b≠c; α≠β≠γ	P	1
7	HEXAGONAL	a=b≠c;α=β=90⁰;γ=120⁰	P	1

6. What are Bravais lattices, mention the 14 Bravais lattices

Ans.

Bravais lattices:

- A three dimensional space lattice is generated by repeated translation of three non-coplanar vectors a, b and c.
- In 1948 Bravais showed that, there are fourteen ways of arranging points in space lattice, under the seven crystal systems to describe crystals.
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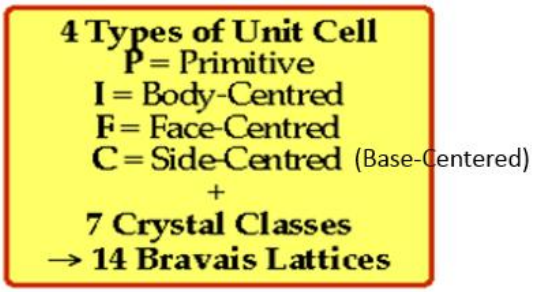

S.N	Crystal System	Shape of UC	Bravais Lattices			
			P	I	F	C
1	Cubic	Cube	✓	✓	✓	
2	Tetragonal	Square Prism (general height)	✓	✓		
3	Orthorhombic	Rectangular Prism (general height)	✓	✓	✓	✓
4	Hexagonal	120° Rhombic Prism	✓			
5	Trigonal	Parallopiped (Equilateral, Equiangular)	✓			
6	Monoclinic	Parallogramic Prism	✓			✓
7	Triclinic	Parallopiped (general)	✓			

7. What are crystalline and non-crystalline soilds?

Crystalline Solids	Amorphous Solids
1. Atoms or molecules have regular periodic arrangements	Atoms or molecules are not arranged in a regular periodic manner. They have random arrangement.
2.They exhibit different magnitudes of physical properties in different directions.	They exhibit same magnitudes of physical properties in different directions.
3.They are anisotropic in nature.	They are isotropic in nature.
4. They exhibit directional properties.	They do not exhibit directional properties.
5.They have sharp melting points.	They do not possess sharp melting points
6. Crystal breaks along regular crystal planes and hence the crystal pieces have regular shape Ex: Copper, Silver, Aluminium etc	Amorphous solids breaks into irregular shape due to lack of crystal plane. Ex: Glass, Plastic, rubber, etc.

8. Define coordination number and packing fraction

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- Simply, co-ordination number of an atom is the number of atoms which it touches.
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9. Write expressions relating r and a for SC, BCC, FCC structures

Nearest neighbour distance

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Atomic radius

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10. Define atomic packing factor, mention its value for SC, BCC and FCC structures

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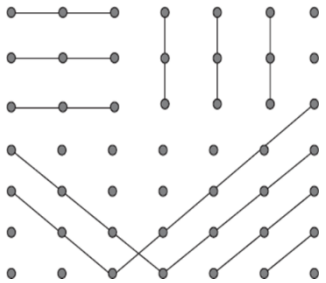


12. What is the building block in a crystal mention its types.

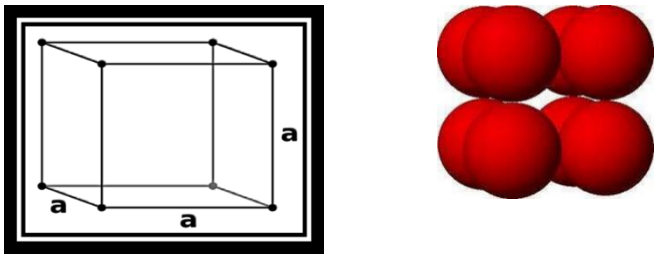
Ans. Unit Cell

- An unit cell is the smallest geometric figure, the repetition of which in three dimensions will give the actual crystal structure.
- Hence, the unit cell may be now defines as 'the smallest fundamental elementary pattern of minimum of atoms (molecules or group of molecules) which represents fully all the characteristics of the crystal'.

Types of Unit cell:

Primitive cell (P):

- Parallelepiped, formed by lattice points only at their corners are called as primitive cell or simple cell.
- The primitive cell is defined as "a unit cell which contains lattice points at corners only'.
- Such cell contains effectively one lattice point per cell, i.e., one lattice point as associated with each primitive cell.
- Example for primitive cell: Simple Cubic unit cell.



Non primitive cell or Multiple Cell:

- If a unit cell contains more than one lattice point then it is called as a multiple cell or non primitive cell.

  Examples for non-primitive cell: BCC and FCC unit cell.

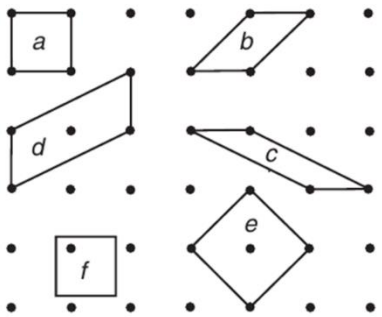


Fig: Primitive and non-primitive unit cells in 2-dimsensions.

13. Define miller indices, obtain miller indices for the plane, a, 2b, 3c

MILLER INDICES

- The Miller index gives a mathematical description to explain lattice directions and lattice planes.
- The Miller Indices are the three smallest possible integers which have the same ratios as the reciprocals of the intercepts of the plane concerned on the three axes.

- a plane making intercepts a, 2b, 3c along X, Y, Z directions.
- The intercepts in multiples of lattice parameters are 1, 2, 3
- The reciprocals of intercepts are $\frac{1}{1}, \frac{1}{2}, \frac{1}{3}$

- Clear these fractions [by multiplying with LCM] to smallest integers having the same ratio as the fractions, enclose these integers in brackets.

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

- So the miller indices are (6, 3, 2)

14. What is interplanar seperation write its expression for an orthogonal system

Interplanar Spacing

- The distance 'd' between successive lattice planes is known as the inter-planar distance.
- The inter-planar distance 'd' involves the axial lengths of the unit cell and the Miller indices of the planes. We shall derive here an expression for d in the case of a cubic system only.
- We know that the three axes of a cubic crystal are mutually perpendicular.
- Let ABC be one of the family of parallel lattice planes in the crystal (Fig).

Let its Miller indices be (hkl) and the intercepts on the crystallographic axes be,

OA = a/h , OB = b/k , and OC = c/l.

The next plane of the set parallel to ABC passes through the origin of the coordinates O (which is not shown in the Fig.).

Therefore, ON, the length of the normal from the origin to the plane is equal to 'd'.

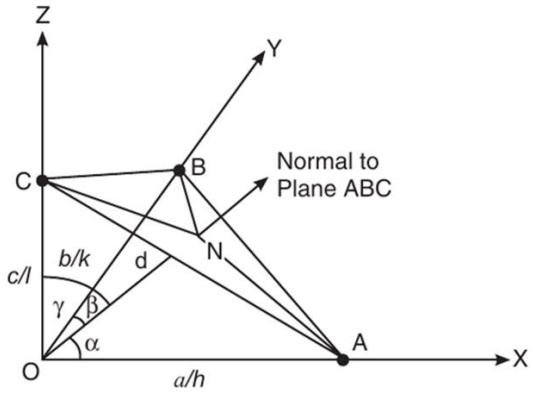


Fig. Determination of interplanar distance in a cubic crystal

Let α, β, and γ be the angles ON makes with the three crystallographic axes respectively.

Then the direction cosines of ON are

$$\cos\alpha = \frac{ON}{OA} = \frac{d}{a/h}$$

$$\cos\beta = \frac{ON}{OB} = \frac{d}{b/k}$$

$$\cos\gamma = \frac{ON}{OC} = \frac{d}{c/l}$$

The sum of the squares of the direction cosines of a line equals unity. Thus,

$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$$

Substituting the values of cosα, cosβ, cosγ, in the above equation,

$$\frac{d^2}{a^2/h^2} + \frac{d^2}{b^2/k^2} + \frac{d^2}{c^2/l^2} = 1$$

$$d^2\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right] = 1$$

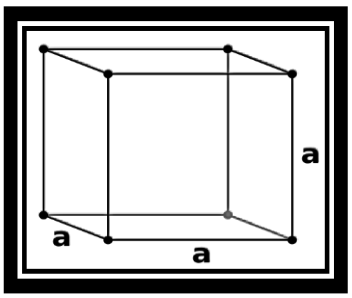
$$d = \left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right]^{-1/2}$$

In case of cubic system, a=b=c. So,

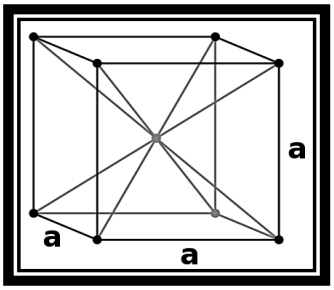
$$d_{hkl} = \frac{a}{\sqrt{(h^2 + k^2 + l^2)}}$$

15. Draw the SC, BCC and FCC structures

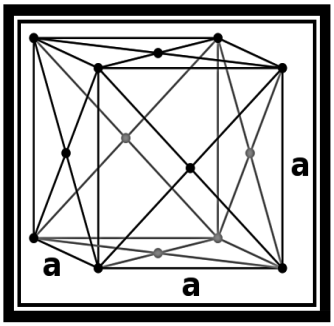
SC



BCC



FCC



16. Obtain the packing fraction of SC sturture

Packing fraction of SC

Volume of one atom (spherical) is = $\frac{4}{3}\pi r^3$ (2)

We know that, the radius of atom in simple cubic is

r = a/2 (3)

Volume of the unit cell (V) = length x breadth x height

We know that for a cubic system, Length = breath = height = a

V = a x a x a

V = a3 ……. (6)

Substitute equation (5) and (6) in equation (1) we get, atomic packing factor (APF) is,

APF = $\frac{\pi a^3/6}{a^3}$

APF = π/6

or APF = 0.52 …… (7)

Therefore, we can say that 52% volume of the unit cell of SC is occupied by atoms and remaining 48% volume is vacant. Thus, the packing density is 52%. Since the packing density is very low, SC has loosely packed structure.

17. Obtain the packing fraction of BCC structure

Packing fraction of BCC

APF = zv/V ……. (1)

In body-centred cubic structure,

The number of atoms per unit cell = 2

Volume of an atom (spherical) is = 4/3 πr^3…… (2)

We know that, the atomic radius of BCC is r =$(a\sqrt{3})/4$…….. (3)

Volume occupied by the total number of atoms per unit cell is

$$zv = 2 \times 4/3\ \pi r^3 \text{ …….. (4)}$$

Substitute equation (3) in (4) we get,

$$zv = \frac{8\pi}{3}\left[\frac{a\sqrt{3}}{4}\right]^3$$

$$zv = \pi a^3 \frac{\sqrt{3}}{8} \text{ …….(5)}$$

Volume of the unit cell for a cubic system is

$$V = a^3 \text{ …….. (6)}$$

Substitute equation (5) and (6) in equation (1) we get,

Atomic pacing factor (APF) = $\frac{\pi a^3 \frac{\sqrt{3}}{8}}{a^3}$

$$APF = \frac{\pi\sqrt{3}}{8}$$

APF = 0.68 …….. (7)

Therefore, we can say that 68% volume of the unit cell of BCC is occupied by atoms and remaining 32% volume is vacant.

18. Obtain the packing fraction of FCC sturture

Packing fraction of FCC

$$APF = \frac{zv}{V} \text{ ……..(1)}$$

In face-centred cubic structure,

The number atoms per unit cell = 4

Volume of atoms is = $\frac{4}{3}\pi r^3$ ……..……. (2)

We know that, the atomic radius of FCC is

$r = \frac{a\sqrt{2}}{4}$ …….……. (3)

Volume occupied by the atoms per unit cell is

$zv = 4 \times \frac{4}{3}\pi r3$ …… (4)

Substitute equation (3) in (4) we get,

$$zv = \frac{16\pi}{3}\left[\frac{a\sqrt{2}}{4}\right]^3$$

$$zv = \frac{16\pi}{3}\left[\frac{a\sqrt{2}}{4}\right]^3$$

$$zv = \pi a^3 \frac{\sqrt{2}}{6} \text{.....(5)}$$

Volume of the unit cell for a cubic system is

$V = a^3$ …… (6)

Substitute equation (5) and (6) in equation (1) we get,

Atomic packing factor (APF) = $\frac{\frac{\pi a^3\sqrt{2}}{6}}{a^3}$

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

APF =0.74 …… (7)

Therefore, we can say that 74% volume of the unit cell of FCC is occupied by atoms and remaining 26% volume is vacant.

19. What are the different lattice arrangements possible in a crystal system?

Crystal Systems:

There are 32 classes of crystals based on geometrical considerations. Taking different symmetries and structures into consideration, all these structures are classified into seven crystal systems. Each system is characterized by the values of a,b,c and α, β, γ.

The seven crystal systems are given as

1.Cubic

2.Tetragonal

3. Orthorhombic

4. Trigonal (or) Rhombohedral

5. Monoclinic

6.Triclinic

7. Hexagonal

20. Draw the four latti ces for a Orthorhombic crystal system

In orthorhombic crystals, the crystal axes are perpendicular to one another. Thus, $\alpha = \beta = \gamma = 90°$.

But the lengths of the edges of unit cell along the three axes are different. That is, $a \neq b \neq c$.

Orthorhombic lattice has four possible types of arrangements, simple (P), base centered (C), body centered (I) and face centered (F).

Ex: Olivine (Mg_2SiO_4), Celestine ($SnSO_4$), Carnalite ($KCl.\ MgCl_2.5H_2O$) etc.,