THE SOLID STATE

PACKING EFFICIENCY

INTERSTICES OR VOIDS OR HOLES IN CRYSTALS

It has been shown that the particles are closely packed in the crystals even than there is some empty space left in between the spheres. This is known as interstices (or interstitial site or holest or empty space or voids).

In three dimensional close packing (CCP & HCP)the interstices are of two types :

(i) Tetrahedral Interstices

(ii) Octahedral Interstices

<u>LOCATING TETRAHEDRAL VOIDS</u>: -

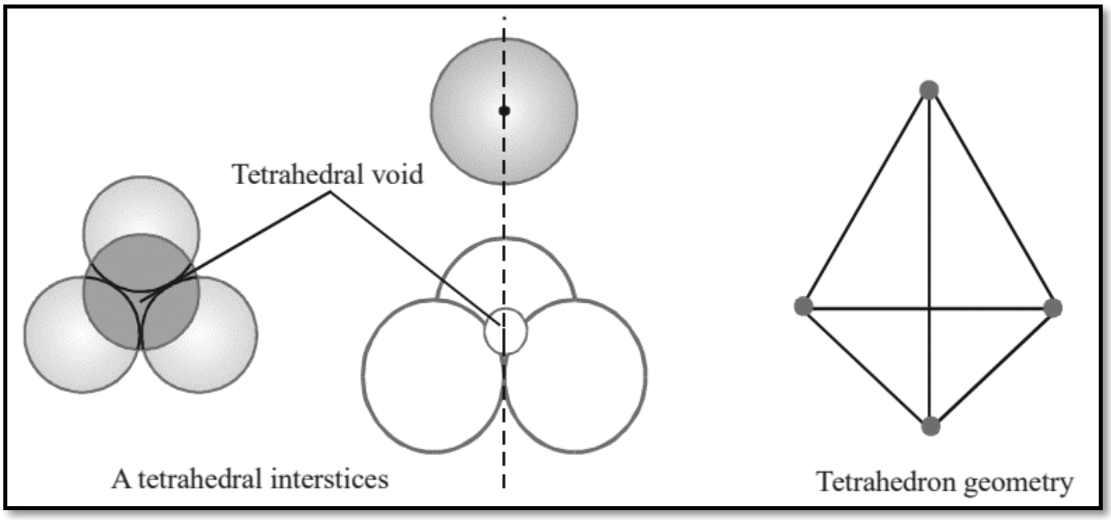
(i) TETRAHEDRAL INTERSTICES:

We have seen that in hexagonal close packing (hcp) and cubic close packing (ccp) each sphere of second layer touches with three spheres of first layer. Thus they, leave a small space in between which is known as tetrahedral site or interstices. or the vacant space between 4 touching spheres is called as tetrahedral void. Since a sphere touches three spheres in the below layer and three spheres in the above layer hence there are two tetrahedral sites associated with one sphere. It may by noted that a tetrahedral site does not mean that the site is tetrahedral in geometry but it means that this site is surrounded by four spheres and the centres of these four spheres lie at the apices of a regular tetrahedron.

In FCC, one corner and it's there face centres form a tetrahedral void

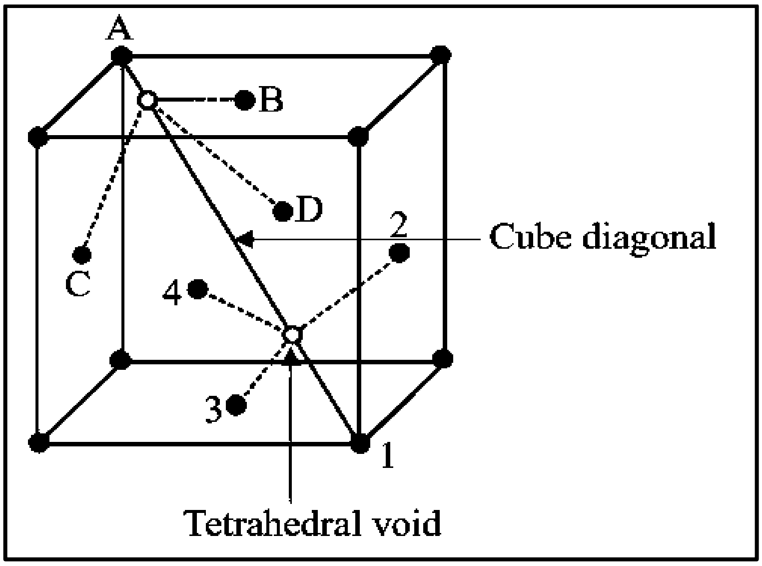
In FCC, two tetrahedral voids are obtained along one cube diagonal. So, in FCC 8 tetrahedral void is present.

In FCC total number of atoms = 4



In FCC total number of tetrahedral voids = 8

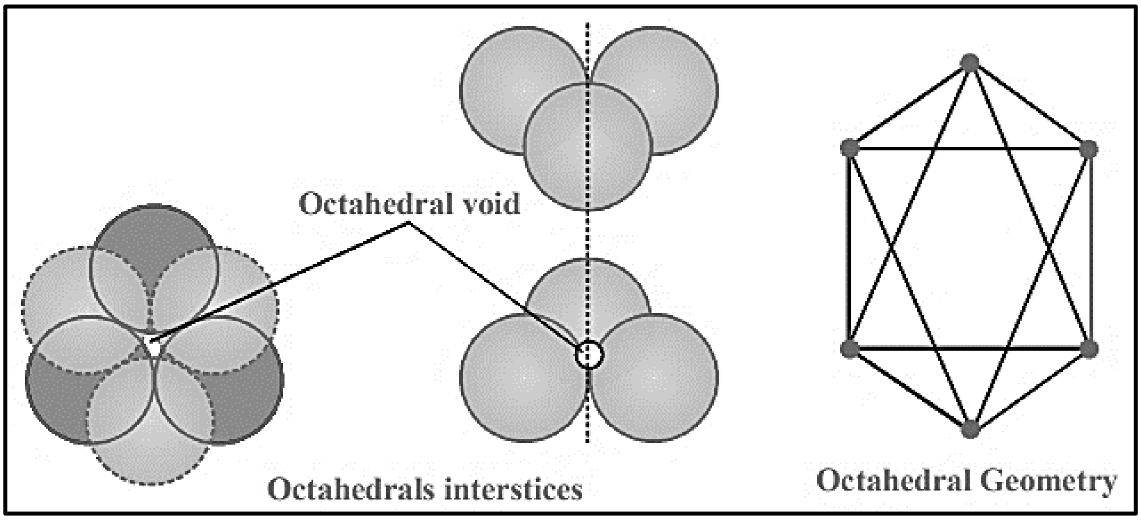
So, we can say that, in 3D close packing 2 tetrahedral voids are attached with one atom



<u>LOCATING OCTAHEDRAL VOIDS IN CCP OR FCC</u>: -

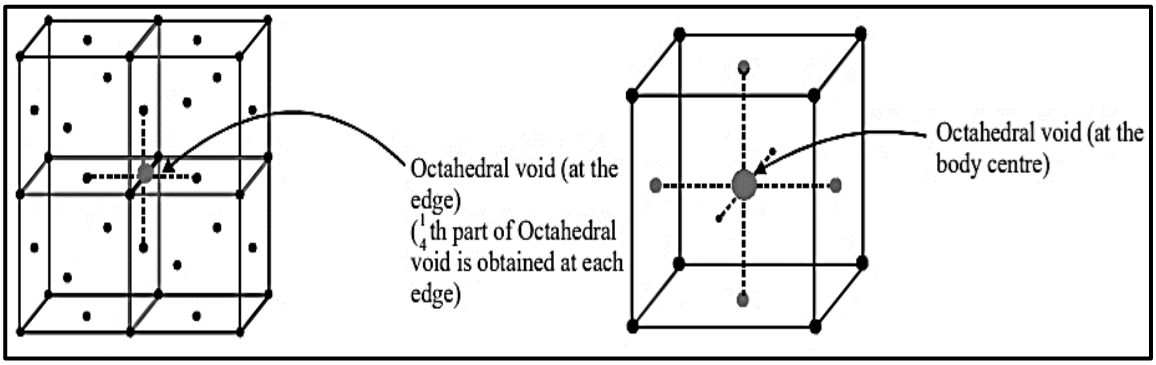
(II) OCTAHEDRAL - INTERSTICES:

Hexagonal close packing (hcp) and cubic close packing (ccp) also form another type of interstices (or site) which is called octahedral site (or interstices). or the vacant space between 6 touching spheres is called as octahedral void. In the figure two layers of close packed spheres are shown. The spheres of first layer are shown by full circles while that of second layer by dotted circles. Two triangles are drawn by joining the centres of three touching spheres of both the layers.



In FCC, 6 face centres form a octahedral void

The apices of these triangles point are in opposite directions. On super imposing these triangles on one another a octahedral site is created. It may be noted that an octahedral site does not mean that the hole is octahedral in shape but it means that this site is surrounded by six nearest neighbour lattice points arranged octahedrally.



In FCC, total number of octahedral voids are $(1 \times 1) + (12 \times \frac{1}{4}) = 1 + 3 = 4$

(Cube centre) (edge)

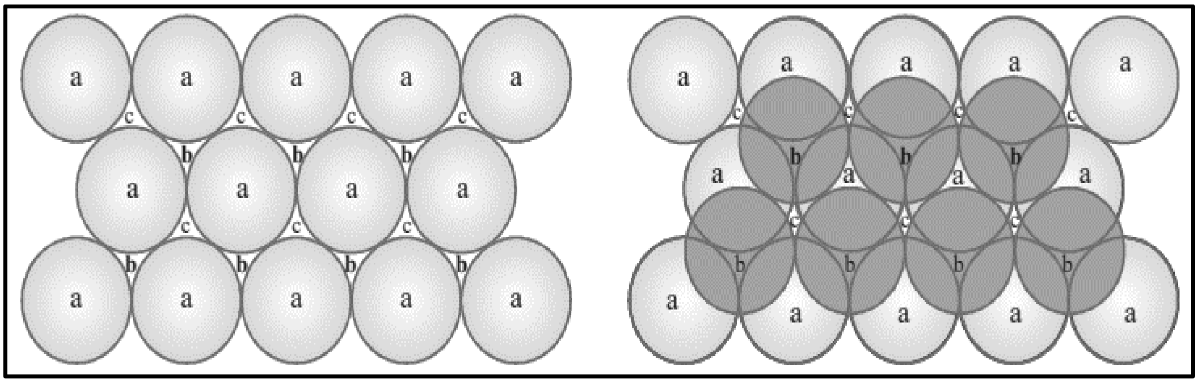
In FCC, number of atoms = 4

In FCC, number of octahedral voids = 4

<u>PACKING IN SOLID - THREE DIMENSIONAL AND ITS TYPES</u>: -

Three Dimensionally close packing:

In hexagonal close packing, there are two types of the voids (open space or space left) which are divided into two sets 'b' and 'c' for convenience. The spaces marked 'c' are curved triangular spaces with tips pointing upwards whereas spaces marked 'b' are curved triangular spaces with tips pointing downwards.

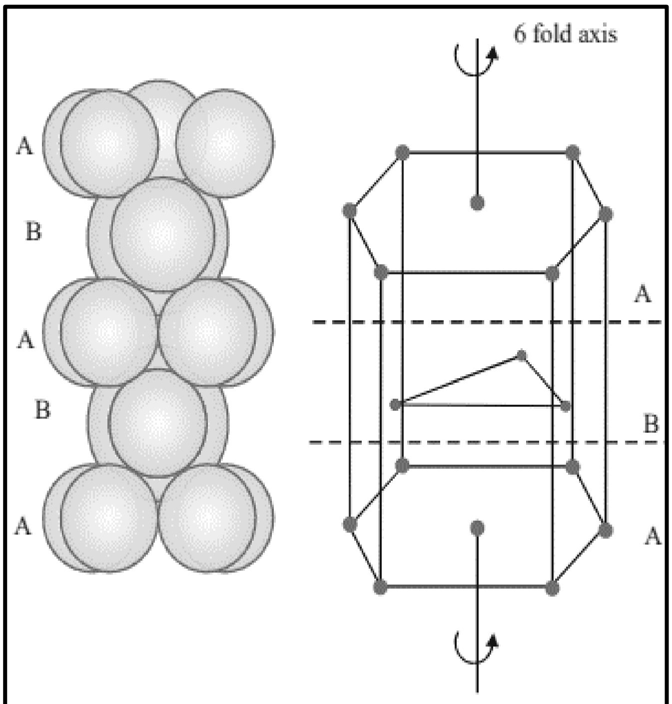


Now we extend the arrangement of spheres in three dimensions by placing second close packed layer (hexagonal close packing) (B) on the first layer (A). The spheres of second layer may place either on space denoted by 'b' or 'c'. It may be noted that it is not possible to place spheres on both types of voids (i.e., b and c). Thus, half of the voids remain unoccupied by the second layer. The second layer also have voids of the types 'b' and in order to build up the third layer,

there are following two ways:

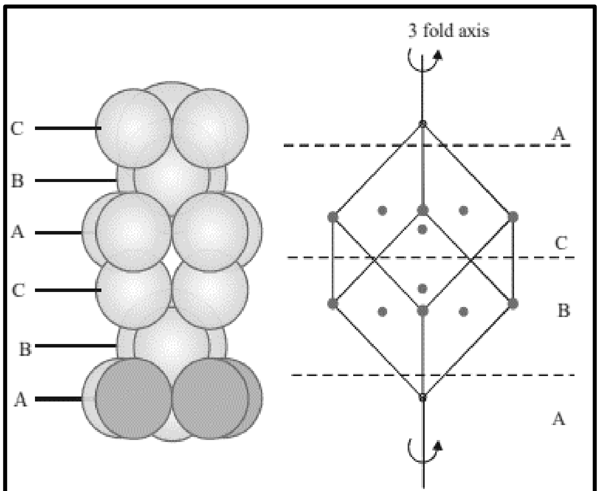
(i) In one way, the spheres of the third layer lie on the spaces of second layer (B) in such a way that they lie directly above those in the first layer(A). In other words, we can say that the third layer becomes identical to the first layer. If this arrangement is continued indefinitely in the same order this represented as AB AB AB ....

This type of arrangement represents hexagonal close packing (hcp) symmetry (or structure), which means that the whole structure has



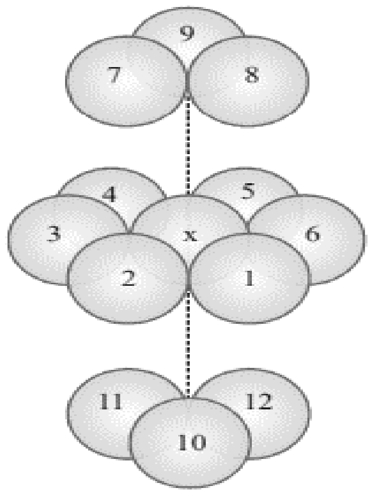
ABABAB ..... or hexagonal close packing (hcp) of spheres only one 6-fold axis of symmetry i.e., the crystal has same appearance on rotation through an angle of 60^0.

(ii) In second way, the spheres of the third layer **(C)** lie on the second layer **(B)** in such a way that they lie over the unoccupied spaces 'C' of the first layer (A). If this arrangement is continuous in the same order this is represented as ABC ABC ABC .... This type of arrangement represents cubic close packed (ccp) structure.



ABCABCA .... or cubic close packing (ccp) of spheres

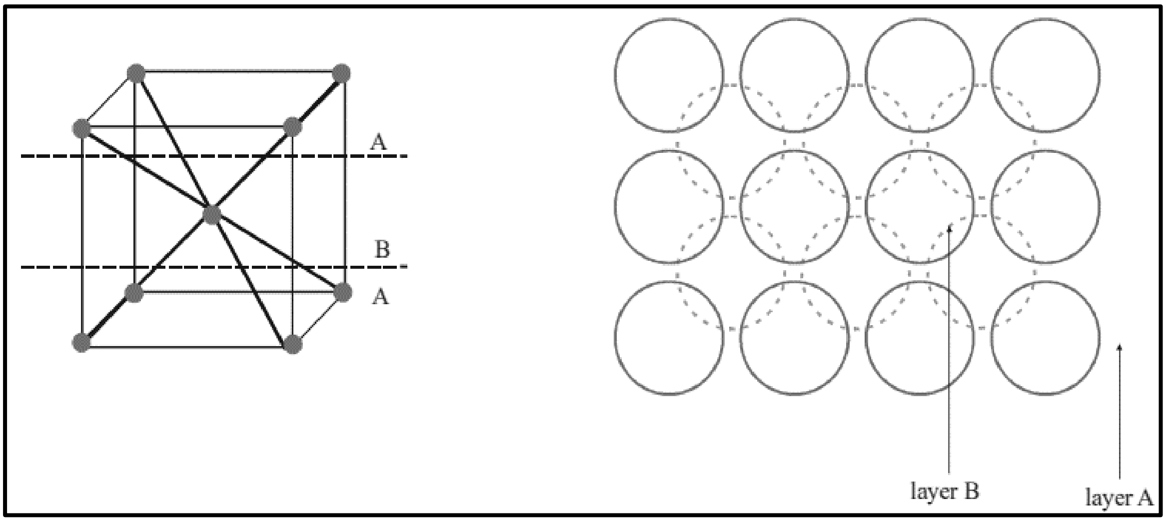
This structure has 3-fold axes of symmetry which pass through the diagonal of the cube. since in this system, there is a sphere at the centre of each face of the unit cell and hence this structure is also known as face-centred cubic (fcc) structure.



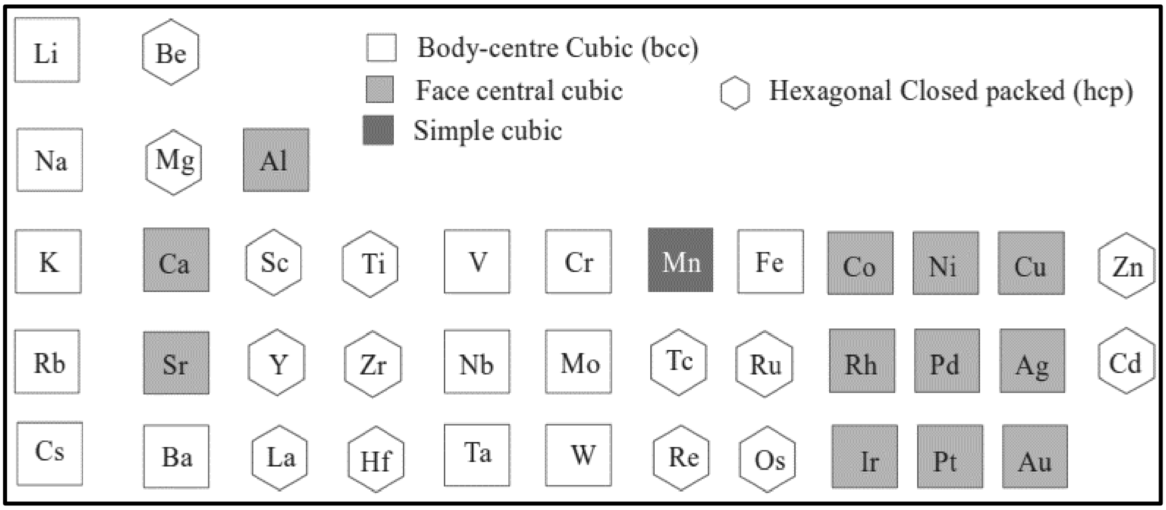
Coordination number of hcp and ccp structurs

It may be noted that in ccp (or fcc) structures each sphere is surrounded by 12 spheres hence the coordination number of each sphere is 12. The spheres occupy 74% of the total volume and 26% of is the empty space in both (hcp and ccp) structures.

(ii) There is another possible arrangement of packing of spheres known as body centred cubic (bcc) arrangement. This arrangement is observed in square close packing (which is slightly opened that hexagonal close packing). In bcc arrangement the spheres of the second layer lie at the space (hollows or voids) in the first layer.



Thus, each sphere of the second layer touches four spheres of the first layer. Now spheres of the third layer are placed exactly about the spheres of first layer. In this way each sphere of the second layer touches eight spheres (four of 1st layer and four of IIIrd layer). Therefore, coordination number of each sphere is 8 in bcc structure. The spheres occupy 68% of the total volume 32% of the volume is the empty space. Some examples of metals with their lattice types and coordination number are given in the following table.



Three-dimensional close packing

CONTENTS	BCC	CCP/FCC	HCP
Type of packing packing but not close packing	ABAB....... close packing	ABCABC ...... close packing	ABAB ......
No. of atoms	2	4	6
Co-ordination no.	8	12	12
Packing efficiency	68%	74%	74%
Examples V & Cr group Fe	IA, Ba Co group, Ni group, Copper group, all inert gases except helium	Ca, Sr, Al d-block elements Be & Mg	Remaining

Note: - Only Mn crystallizes in S.C.C.