PACKING EFFICIENCY

Interstices or Voids or Holes in Crystals

It has been demonstrated that particles in crystals are tightly packed, yet there exists some residual empty space between the spheres. This space is commonly referred to as interstices, interstitial sites, holes, empty space, or voids.

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

(i) Tetrahedral Interstices

(ii) Octahedral Interstices

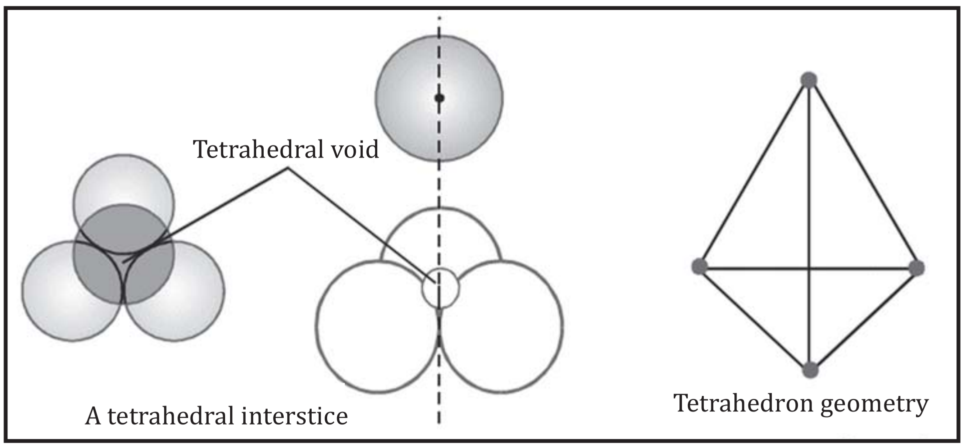
Locating Tetrahedral Voids

(i) Tetrahedral Interstices

We observed in hexagonal close packing (hcp) and cubic close packing (ccp) that each sphere in the second layer makes contact with three spheres from the first layer. This interaction creates a small space in between, referred to as a tetrahedral site or interstice. Alternatively, the vacant area between four touching spheres is known as a tetrahedral void. Since a sphere touches three spheres in the layer below and three spheres in the layer above, each sphere is associated with two tetrahedral sites. It's important to note that a tetrahedral site does not necessarily have a tetrahedral geometry; rather, it means that the site is surrounded by four spheres, and the centers of these four spheres lie at the apices of a regular tetrahedron.

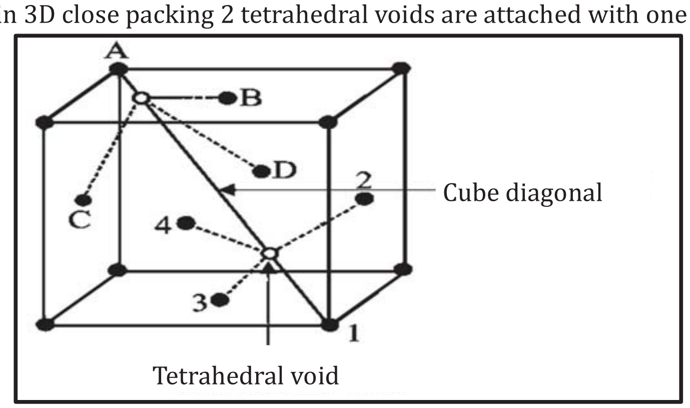
In the face-centered cubic (FCC) structure, a tetrahedral void is formed by one corner and its three face centers. Moreover, two tetrahedral voids are present along one cube diagonal in FCC. Therefore, there are a total of 8 tetrahedral voids in FCC.

In FCC total number of atoms = 4



In FCC total number of tetrahedral voids = 8

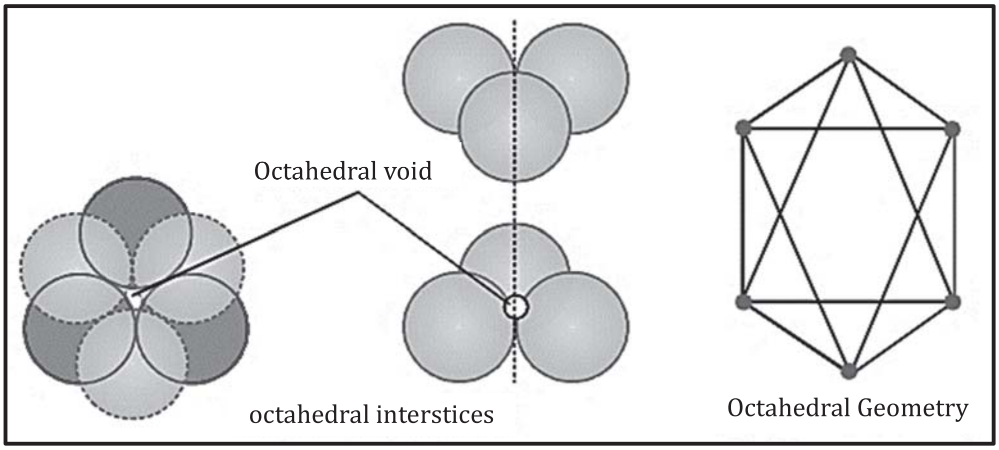
So, we can say that, in 3D close packing 2 tetrahedral voids are attached with one atom



Locating Octahedral Voids in CCP or FCC

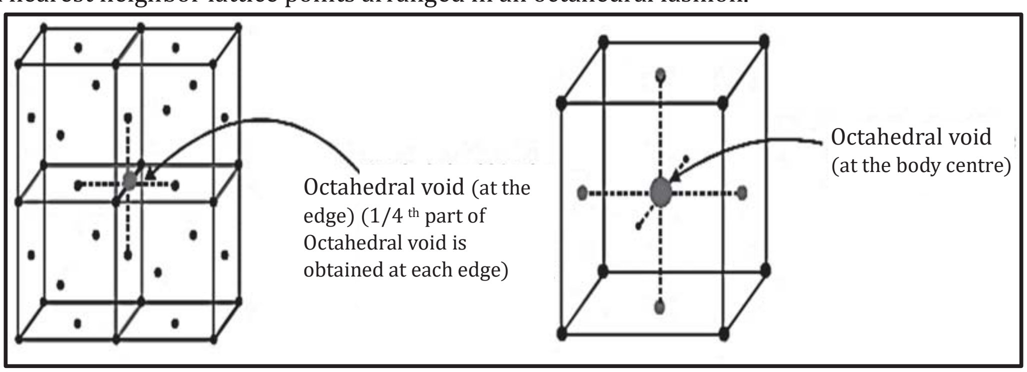
(ii) Octahedral - Interstices

Hexagonal close packing (hcp) and cubic close packing (ccp) also give rise to another type of interstice or site known as an octahedral site. Alternatively, the empty space between six touching spheres is referred to as an octahedral void. The illustration depicts two layers of closely packed spheres, with full circles representing those in the first layer and dotted circles representing those in the second layer. Two triangles are formed by connecting the centers of three touching spheres from both layers.



In FCC, 6 face centres form a octahedral void

The apices of these triangles are oriented in opposite directions. When these triangles are superimposed on each other, they create an octahedral site. It's important to clarify that an octahedral site does not imply that the void is shaped like an octahedron; rather, it means that this site is encircled by six nearest neighbor lattice points arranged in an octahedral fashion.



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

(Cube centre) (edge)

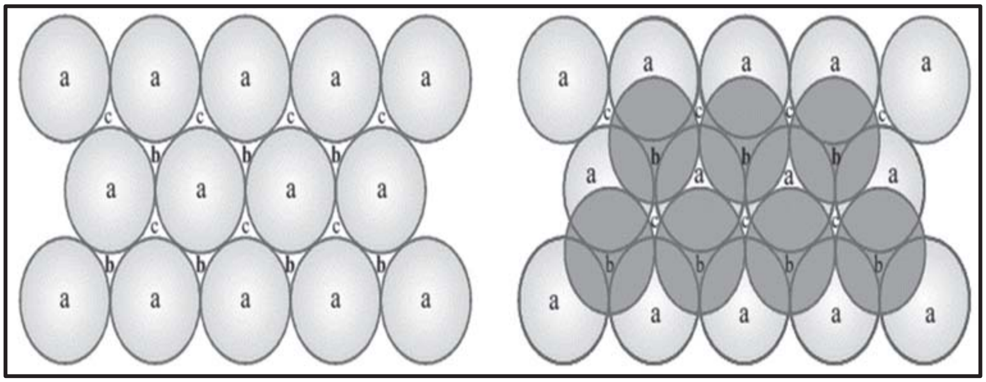
In FCC, number of atoms = 4

In FCC, number of octahedral voids = 4

Packing In Solid - Three Dimensional and Its Types

Three Dimensionally close packing

Within hexagonal close packing, two categories of voids, denoted as 'b' and 'c,' exist for convenience. Spaces labeled 'c' are curved triangular areas with tips pointing upwards, while spaces marked 'b' are curved triangular spaces with tips pointing downwards.

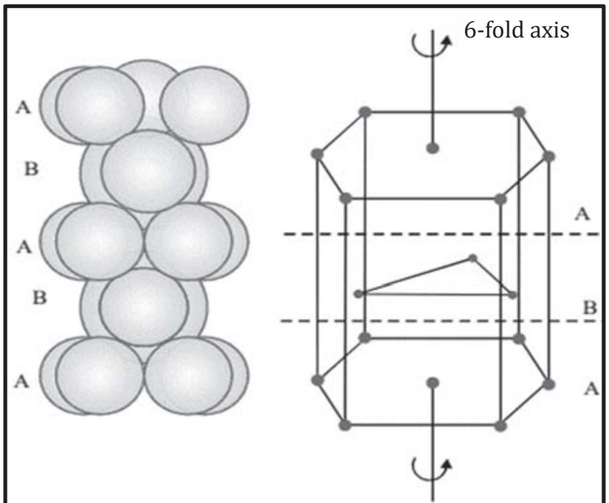


Expanding the arrangement of spheres into three dimensions involves adding a second close-packed layer (hexagonal close packing) (B) onto the first layer (A). The spheres in the second layer can be positioned in spaces labeled as 'b' or 'c.' Importantly, it is not feasible to place spheres in both types of voids (i.e., b and c). As a result, half of the voids in the second layer remain unoccupied. Additionally, the second layer also contains voids of type 'b,' setting the foundation for constructing the third layer.

There are following two ways

(i) In one approach, the spheres of the third layer are positioned on the spaces of the second layer (B) in a manner that aligns directly above those in the first layer (A). Alternatively, we can express this as the third layer becoming identical to the first layer. If this sequence continues consistently, it is denoted as AB, AB, AB, and so forth.

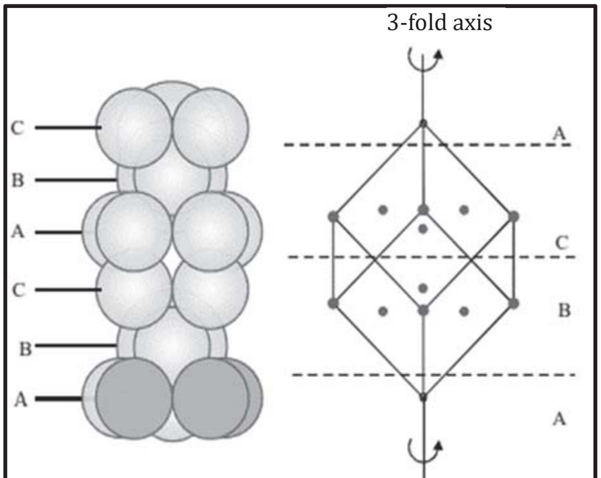
This particular arrangement signifies hexagonal close packing (hcp) symmetry or structure, indicating that the entire structure possesses only one 6-fold axis of symmetry. In other words, the crystal maintains the same appearance when rotated through an angle of 60 degrees.



ABABAB…. or hexagonal close packing (hcp) of spheres

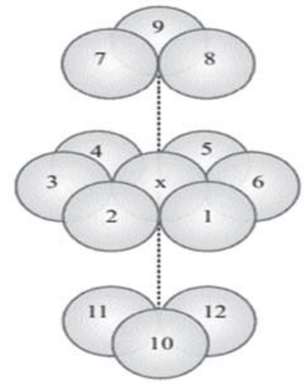
(ii) Alternatively, in the second approach, the spheres of the third layer (C) are positioned on the second layer (B) in such a manner that they align over the unoccupied spaces labeled 'C' in the first layer (A). If this sequence persists in the same order, it is denoted as ABC, ABC, ABC, and so on. This arrangement characterizes a cubic close-packed (ccp) structure.

The ccp structure possesses 3-fold axes of symmetry that pass through the diagonal of the cube. Because there is a sphere at the centre of each face in the unit cell, this structure is also recognized as a face-centered cubic (fcc) structure.



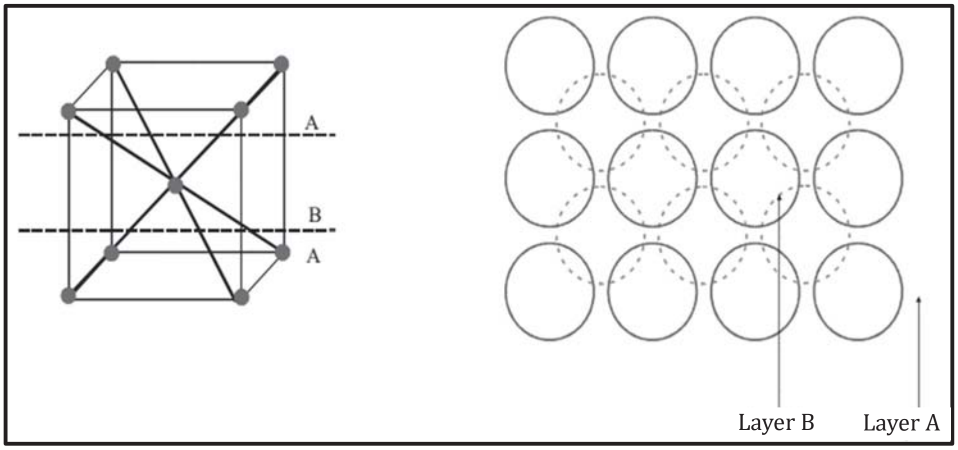
ABCABCA…. or cubic close packing (hcp) of spheres

It's important to observe that in ccp (or fcc) structures, each sphere is encompassed by 12 neighboring spheres, resulting in a coordination number of 12 for each sphere. The spheres occupy 74% of the total volume, leaving 26% as empty space in both hcp and ccp structures.



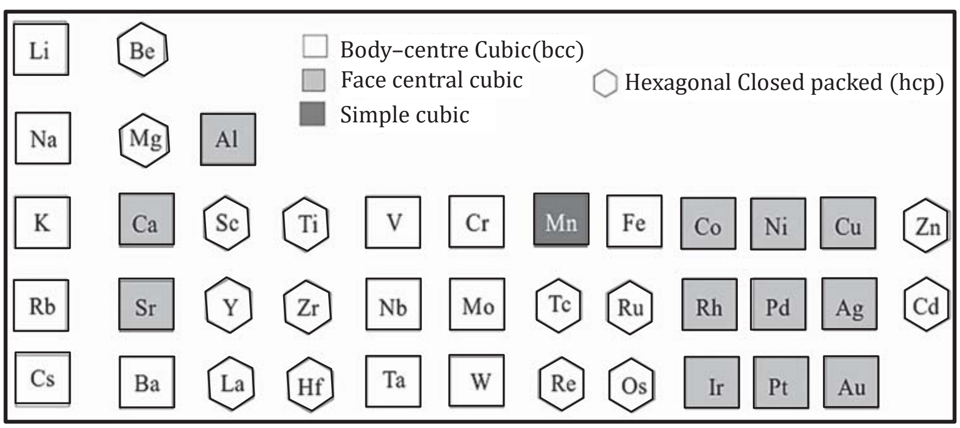
Coordination number of hcp and ccp structures

(iii) An alternative packing arrangement of spheres is called the body-centered cubic (bcc) arrangement. This arrangement is present in square close packing, which is slightly less closed than hexagonal close packing. In the bcc arrangement, the spheres of the second layer are positioned within the voids or hollow spaces of the first layer.



Consequently, each sphere in the second layer makes contact with four spheres from the first layer. Subsequently, the spheres in the third layer are precisely positioned above those in the first layer. As a result, each sphere in the second layer is in contact with eight spheres (four from the first layer and four from the third layer). Hence, the coordination number for each sphere is 8 in the bcc structure. The spheres occupy 68% of the total volume, with 32% of the volume being empty space.

Examples of metals, along with their lattice types and coordination numbers, are provided in the table below.



Three-dimensional close packing

CONTENTS	BCC	CCP/FCC	HCP
Type of 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: Solely manganese exhibits a simple cubic crystal structure when it crystallizes.