STRUCTURE OF CUBIC

Cubic system

The cubic crystal structure is the simplest type and the atoms can take positions at the corners, faces and also at the centre of the cube. Based on the positions of the atom in the cubic system, it can be classified in to three types. They are,

1. Simple Cubic (SC) or Primitive(P)
2. Body Centred Cubic (BCC) and
3. Face Centred Cubic (FCC)

SIMPLE CUBIC STRUCTURE (SC)

NUMBER OF ATOMS PER UNIT CELL

SC is the simplest and easiest crystal structure. A SC unit cell consists of 8 corner atoms. Each and every corners is shared by eight adjacent unit cells. Therefore,

Number of atoms per unit cell= $8 \times \frac{1}{8} = 1$ atom

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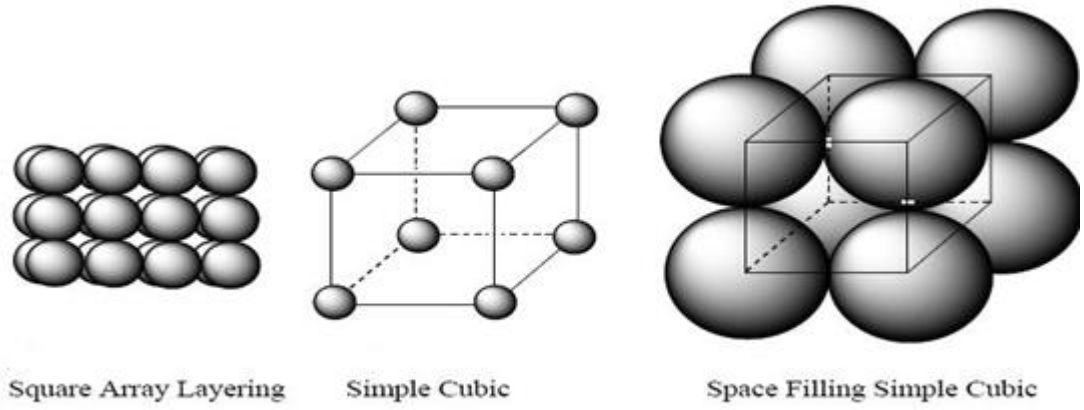
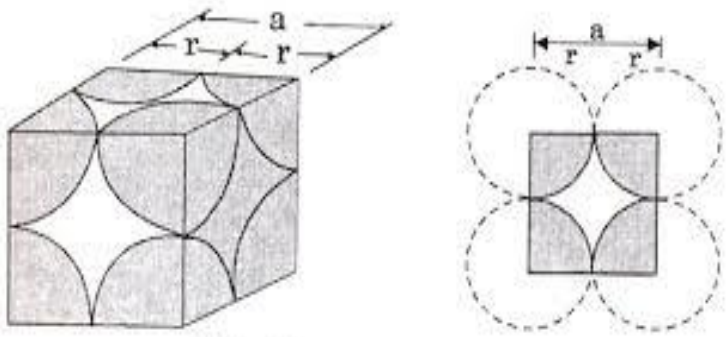


Square Array Layering Simple Cubic Space Filling Simple Cubic

ATOMIC RADIUS

The unit cell has atoms only at the coners of the cube. Let ‘a’ be the side of the unit cell. From fig, $2r = a$

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

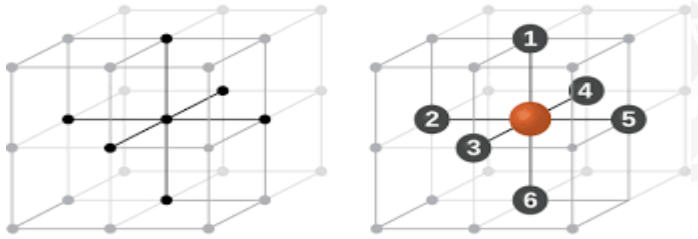


Calculation of Atomic Radius - SC

CO-ORDINATION NUMBER

Each corner atom touches four atoms in its horizontal plane. It also in touches with two more atoms, one above it and another below it. Therefore,

the coordination number= 4+2=6



ATOMIC PACKING FACTOR

$$APF = \frac{Number\ of\ atoms\ per\ unit\ unit\ cell \times cell\ Volume\ of\ one\ atom}{volume\ of\ the\ unit\ cell}$$

$$\text{APF} = \frac{1 \times \frac{4}{3}\pi r^3}{a^3} \qquad \{\therefore r = \frac{a}{2}\}$$

$$= \frac{1 \times \frac{4}{3}\pi \left[\frac{a}{2}\right]^3}{a^3} = \frac{\pi}{6} = 0.52$$

$$APF = 52\%$$

Therefore 52% of the volume is occupied by atoms and remaining 48% is vacant in SC structure. Since packing density is ver low, SC has loosely packed structure. Example: Po

BODY CENTERED CUBIC STRUCTURE (BCC)

NUMBER OF ATOMS PER UNIT CELL

BCC structure has 8 corner atoms and one body centered atom. In a BCC structure, the atoms touch along the diagonals of the body. Each and every corners is shared by eight adjacent unit cells. The number of corner atoms per unit cell= $8 \times \frac{1}{8} = 1$ atom. One full atom present at the body centre of the unit cell.

Therefore Number of atoms per unit cell= $1+1=2$ atoms

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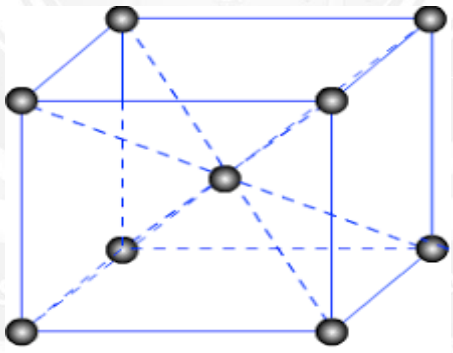


Body Centred

ATOMIC RADIUS

In a BCC structure, the atoms touch along the diagonals of the body. The unit cell has atoms only at the coners of the cube. Let 'a' be the side of the unit cell.

From fig, Diagonal length $AH = r + 2r + r = 4r$ and $DH = a$

In ΔDFG, $AH^2 = AD^2 + DH^2$ ..... (1)

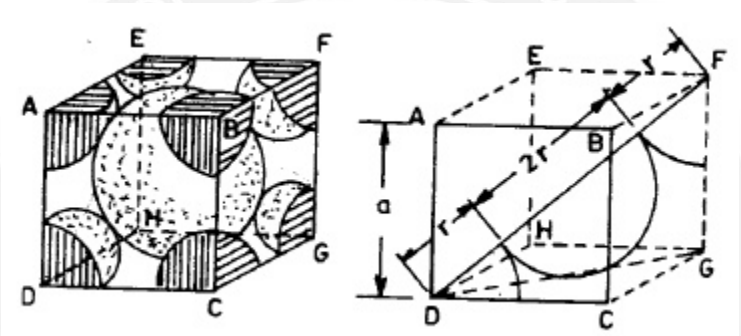
In $\Delta DBD,\ AD^2 = AB^2 + BD^2 = a^2 + a^2 = 2a^2$

$$(1) \rightarrow (4r)^2 = 2a^2 + a^2$$

$$16r^2 = 3a^2$$

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

$$\boxed{r = \frac{\sqrt{3}a}{4}}$$



CO-ORDINATION NUMBER

BCC structure has 8 corner atoms and one body centered atom. A body centered atom is surrounded by eight corner atoms. Therefore, the coordination number= 8

ATOMIC PACKING FACTOR

$$APF = \frac{Number\ of\ atoms\ per\ unit\ unit\ cell \times cell\ Volume\ of\ one\ atom}{volume\ of\ the\ unit\ cell}$$

$$\text{APF} = \frac{2 \times 4/3\,\pi r^3}{a^3} \qquad \{\because r = \frac{\sqrt{3}a}{4}\}$$

$$= \frac{2 \times 4/3\,\pi\left[\sqrt{3}a/4\right]^3}{a^3} = \frac{\sqrt{3}\pi}{8} = 0.68$$

$$\boxed{APF = 68\%}$$

This shows that 68% of the volume is occupied by atoms and remaining 32% is vacant in BCC structure. Example: Na

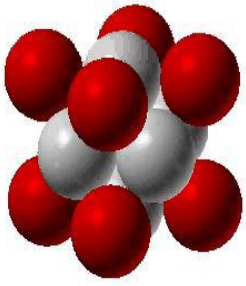
FACE CENTERD CUBIC (FCC) STRUCTURE

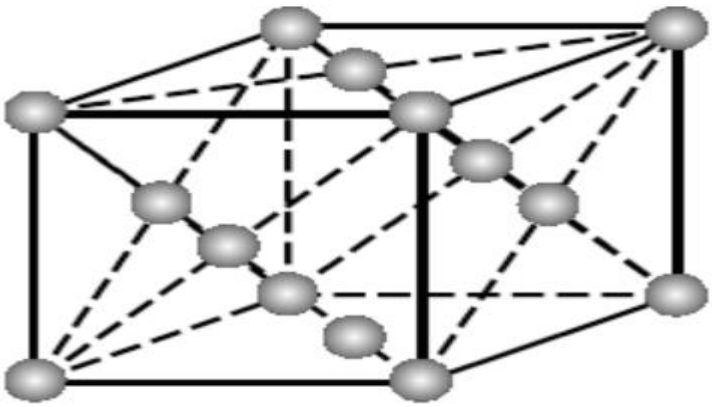
NUMBER OF ATOMS PER UNIT CELL

The atoms in a FCC unit cell touches along the face diagonal. Each and every corner atom is shared by eight adjacent unit cells. Therefore each and every corner atom contributes 1/8 of its part to one unit cell. So the total number of atoms contributed by the corner atoms is $8 \times \frac{1}{8} = 1$ atom.

Two unit cells share each and every face centered atom. Therefore, the contribution of a face centered atom to unit cell is 1/2. So, the total number of atoms contributed by the face centred atoms = $\frac{1}{2} \times 6 = 3$ atoms.

Hence the total number of atoms present in a FCC unit cell = 1+3 = 4.

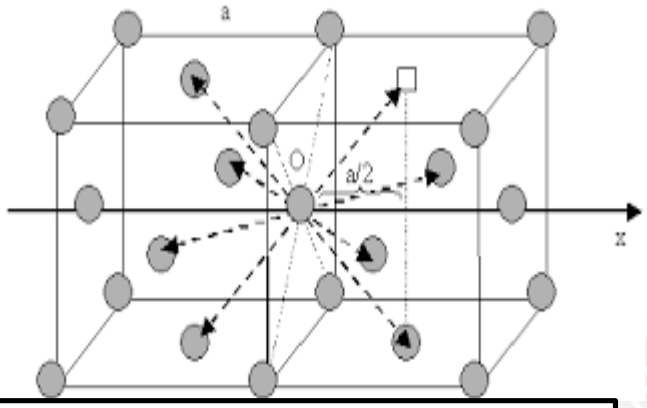




COORDINATION NUMBER

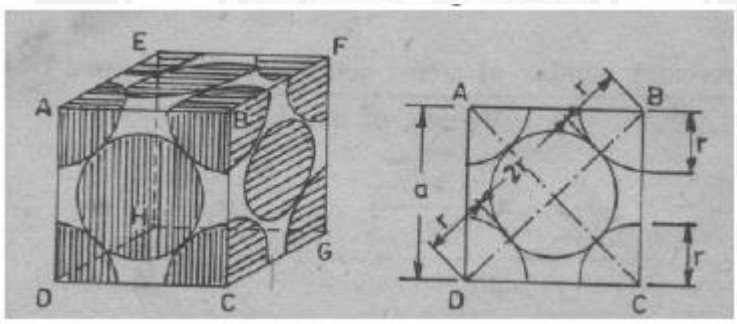
In its own plane it touches four face centered atoms. The face centered atoms are its nearest neighbors. In a plane, which lies just above this corner atom, it has four more face

centered atoms as nearest neighbors. Similarly, in a plane, which lies just below this corner atom it has yet four more face centered atoms as its nearest neighbors. Therefore the number of nearest neighbours i.e.,



Co-ordination number for FCC unit cell = 4+4+4 = 12

ATOMIC RADIUS (R)



The atoms in a FCC unit cell touches along the face diagonal. Let 'a' be the side of the unit cell.

From fig, Diagonal length $DB = r + 2r + r = 4r$ and $DC = a$

In ΔDBC, $DB^2 = DC^2 + CB^2$ ..... (1)

$$(1) \rightarrow (4r)^2 = a^2 + a^2$$

$$16r^2 = 2a^2$$

$$r^2 = \frac{2a^2}{16}$$

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

ATOMIC PACKING FACTOR

$$APF = \frac{Number\ of\ atoms\ per\ unit\ unit\ cell \times cell\ Volume\ of\ one\ atom}{volume\ of\ the\ unit\ cell}$$

$$\text{APF} = \frac{4 \times \frac{4}{3}\pi r^3}{a^3} \qquad \{\because r = \frac{a}{2\sqrt{2}}\}$$

$$= \frac{4 \times \frac{4}{3}\pi\left[\frac{a}{2\sqrt{2}}\right]^3}{a^3} = \frac{\pi}{3\sqrt{2}} = 0.74$$

$$APF = 74\%$$

Thus 74 percent of the volume of the FCC unit cell is occupied by atoms and the remaining 26 percent volume of the unit cell is vacant or void space.

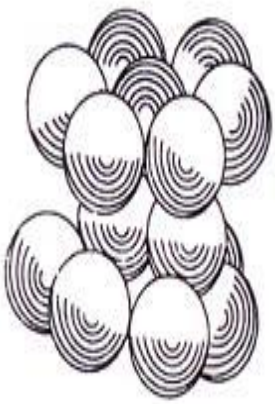
HEXAGONAL CLOSED PACKED STRUCTURE

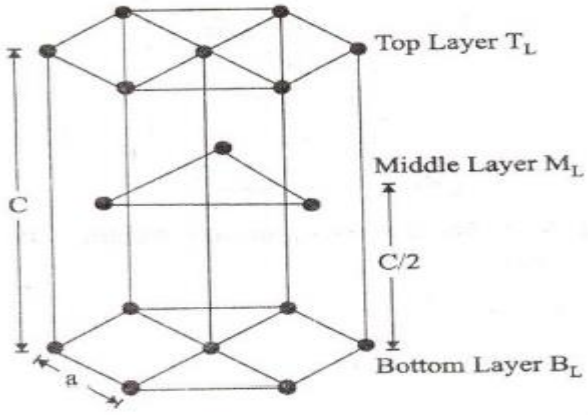
NUMBER OF ATOMS PER UNIT CELL

It consists of three layers of atoms. The bottom layer has six corner atoms and one face centred atom. The middle layer has three full atoms. The upper layer has six corner atoms and one face centred atom.

The contribution of top layer atoms= $(6 \times \frac{1}{6} + 2 \times \frac{1}{2}) = \frac{3}{2}$ atoms

The contribution of top layer atoms= $(6 \times \frac{1}{6} + 2 \times \frac{1}{2}) = \frac{3}{2}$ atoms





The number of atoms present in the middle layer =3

Hence total number of atoms present in an HCP unit cell $= \frac{3}{2} + \frac{3}{2} + 3 = 6$ atoms

CO-ORDINATION NUMBER (CN)

The face centered atom touches 6 corner atoms in its plane. The three middle layer atoms in the plane just below it and 3 middle layer atoms in the plane just above it. Hence the

coordination number is 6+3+3=12

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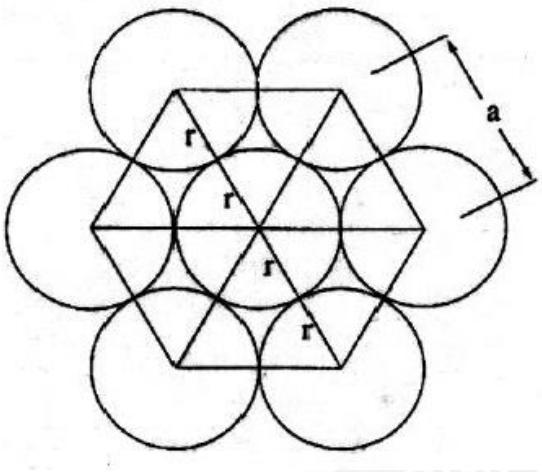
ATOMIC RADIUS (R)

Consider any two corner atoms. Each and every corner atom touches each other. Therefore a = 2r**.**

$$r = a/2$$



CALCULATION OF AXIAL (C/A) RATIO

Let c be the height of the unit cell and 'a' be the lattice constant of the unit cell. The body atoms lie in a horizontal plane at height $c/2$ from the bottom layer. The atomic radius $r = a/2$

From $\Delta ABA'$, $Cos30^\circ = \frac{AA'}{AB}$

$$AA' = AB \times Cos30^\circ = a\frac{\sqrt{3}}{2}$$

From fig, X is orthocenter

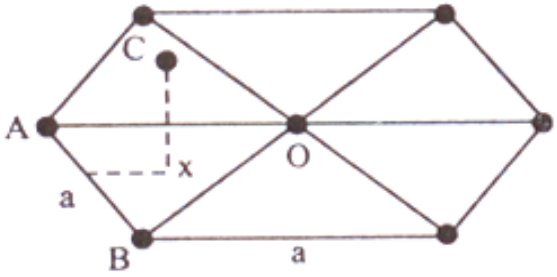
$AX = \frac{2}{3} \times AA' = \frac{2}{3} \times a\frac{\sqrt{3}}{2} = \frac{a}{\sqrt{3}}$ From fig, CX=c/2 and AC=a

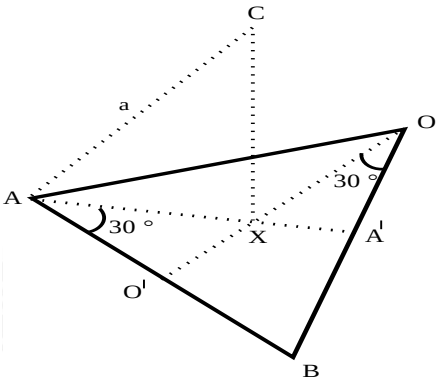
ΔAXC, $AC^2 = AX^2 + CX^2$,

$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2$ $a^2 = \frac{a^2}{3} + \frac{c^2}{4}$ $a^2 - \frac{a^2}{3} = \frac{c^2}{4}$

$\frac{3a^2 - a^2}{3} = \frac{c^2}{4}$ $\frac{2a^2}{3} = \frac{c^2}{4}$ $\frac{c^2}{a^2} = \frac{8}{3}$

$$\frac{c}{a} = \sqrt{\frac{8}{3}} = 1.633$$





ATOMIC PACKING FACTOR

Number of atoms per unit cell = 6

Volume of one atom $\frac{4\pi r^3}{3} = \frac{4\pi}{3}\left(\frac{a}{2}\right)^3 = \frac{4\pi}{3}\frac{a^3}{8} = \frac{\pi a^3}{6}$ $[\because r = \frac{a}{2}]$

Area of the $\Delta AOB = \frac{1}{2} \times BO \times AY = \frac{1}{2} a \times \frac{\sqrt{3}}{2} a = \frac{\sqrt{3}}{4} a^2$

Area of the base =6 × area of $\Delta AOB = 6 \times \frac{\sqrt{3}}{4} a^2 = \frac{3\sqrt{3}}{2} a^2$

Volume of the unit cell =Area of the base × height of the unit cell

$$= \frac{3\sqrt{3}}{2} a^2 \times c$$

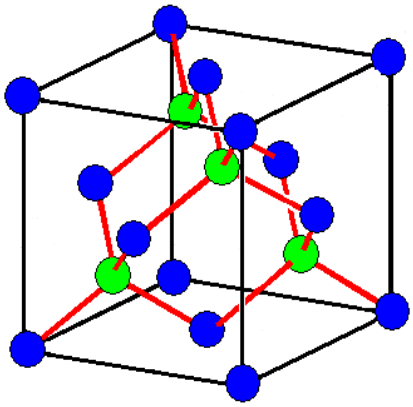
$$APF = \frac{6 \times \frac{\pi a^3}{6}}{\frac{3\sqrt{3}}{2} a^2 c} = \frac{2\pi}{3\sqrt{3}}\left(\frac{a}{c}\right) = \frac{\pi}{3\sqrt{2}}$$

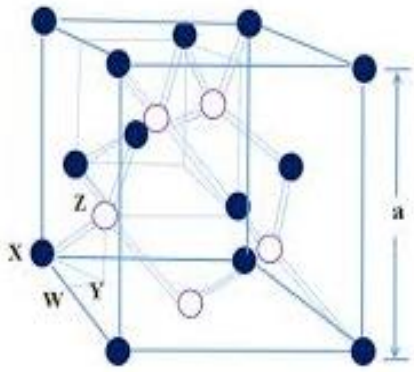
$\therefore APF = 74\%$

Since the APF is 74%, it is a closely packed structure. Mg, Zn and Cd crystallize HCP structure.

1. DIAMOND CUBIC STRUCTURE

Diamond is one of the allotropic forms of carbon. In diamond, carbon atoms are arranged tetrahedrally. Each carbon is attached to four other carbon atoms 1.544 A away with a



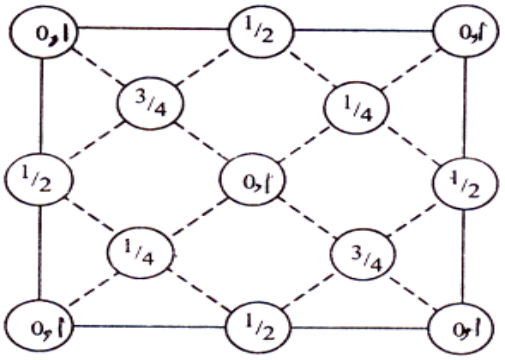


C-C-C bond angle of 109.5°. Diamond structure is formed due to the combination of two interpenetrating FCC sub lattices having the origin (000) and $(a/4, a/4, a/4)$ along the body diagonal.

NUMBER OF ATOMS PER UNIT CELL

Number of atoms per unit cell in diamond carbon atoms are present at three different positions of the unit cell.

- The corner atoms represented by 'C'. There are corner atoms in the unit cell. Each corner atom is shared by 8 unit cells. The total number of corner atoms per unit cell $= 8 \times 1/8 = 1$ atom

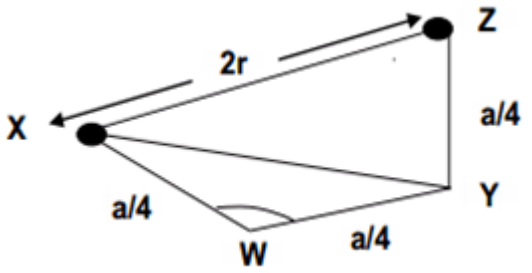


- Face centered atoms represented by 'F'. There are 6 face centered atoms. Each face centered atom is shared by 2 unit cells. Number of face centered atoms per unit cell= $6 \times 1/2 = 3$ atoms
- Number of atoms present inside the unit cell= 4 atoms

Total number of atoms per unit cell= 1+3+4= 8 atoms

Atomic Radius (R)

The corner atoms and face centered atoms don't touch each other. But both the corner atoms and face centered atoms have direct contact with the 4 atoms present inside the unit cell.



From fig,

$$XZ^2 = XZ^2 + WY^2$$

$$XZ^2 = XW^2 + WY^2 + YZ^2$$

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

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

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

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

CO-ORDINATION NUMBER

The co-ordination number is the nearest neighboring atom to a particular atom. The four atoms present inside the unit cell are the nearest neighbors for the corner atom.

The co-ordination number =4

ATOMIC PACKING FACTOR

$$APF = \frac{Number\ of\ atoms\ per\ unit\ unit\ cell \times cell\ Volume\ of\ one\ atom}{volume\ of\ the\ unit\ cell}$$

$$\text{APF} = \frac{8\times \frac{4}{3}\pi r^3}{a^3} \qquad \{\therefore r = \frac{a\sqrt{3}}{8}\}$$

$$= \frac{8\times \frac{4}{3}\pi\left[\sqrt{3}\,\frac{a}{8}\right]^3}{a^3} = \frac{\pi\sqrt{3}}{16} = 0.34$$

$$\boxed{APF = 34\%}$$

The APF is 34%. Since the packing density is very low, it is a loosely packed structure.