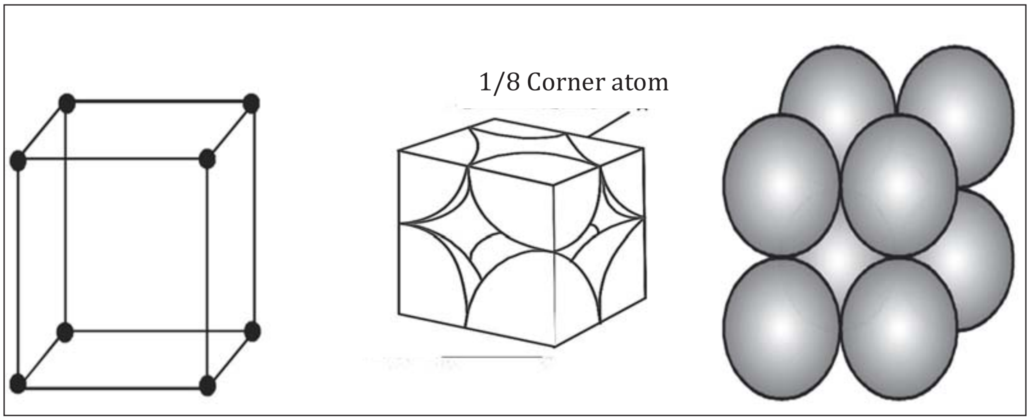
NUMBER OF ATOMS IN A UNIT CELL

Simple Cubic Unit Cell/Primitive/Basic Unit Cell

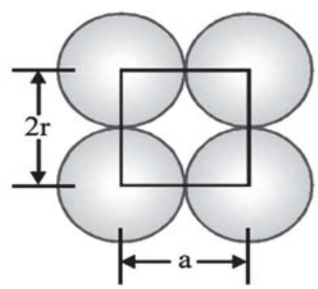
A unit cell with lattice points only at the corners is known as a primitive or simple unit cell. In this case, there is one atom at each of the eight corners of the unit cell. Considering an atom at one corner as the center, it will be observed that this atom is surrounded by six equidistant neighbors (atoms), resulting in a coordination number of six. If 'a' is the side of the unit cell, then the distance between the nearest neighbors will be equal to 'a'.



(a) **Relationship between edge length 'a' and atomic radius 'r':**

$a = 2r$

i.e. $r = \frac{a}{2}$ (One face of SCC)



(b) **Number of atoms present in unit cell**

In this case one atom or ion lies at each corner. Hence simple cubic unit cell contains a total of $\frac{1}{8} \times 8 =$ 1 atom or ion/unit cell.

(c) **Packing efficiency (P. E.)**

$$\text{P.E.} = \frac{\text{Volume occupied by atoms present in unit cwll}}{\text{Volume of unit cwll}} = \frac{n \times \frac{4}{3}\pi r^3}{V} \quad [\because \text{Volume of atom} = \frac{4}{3}\pi r^3]$$

$$\text{P.E.} = \frac{\text{Volume occupied by atoms present in unit cwll}}{\text{Volume of unit cwll}}$$

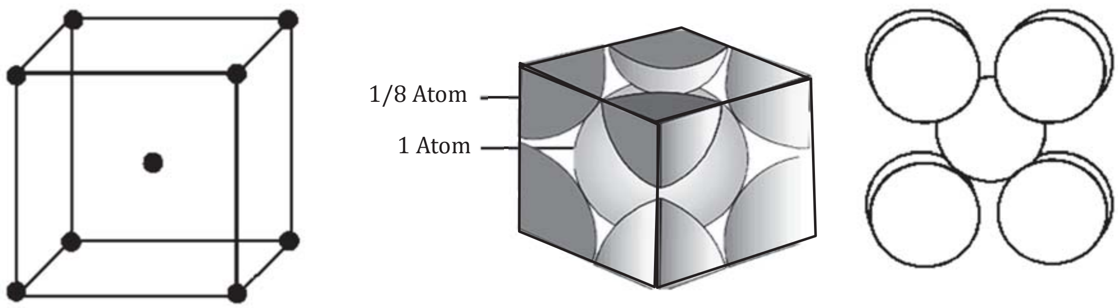
For, $$\text{P.E.} = \frac{1 \times \frac{4}{3} \times \pi \left(\frac{a}{2}\right)^3}{a^3} \quad [\because r = \frac{a}{2} \text{ and } V = a^3, n=1]$$

$$\text{SCC:} = \frac{\pi}{6} = 0.524 \text{ or } 52.4\%$$

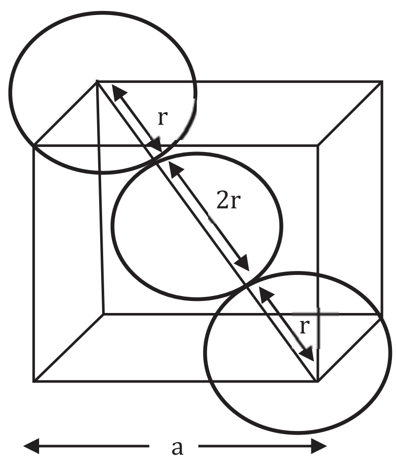
Body Centered Cubic (B.C.C.) CELL

A unit cell that incorporates a lattice point at the body centre, in addition to lattice points at each corner, is termed a body-cantered unit cell. In this arrangement, the central atom is encircled by eight equidistant atoms, resulting in a coordination number of eight.

The nearest distance between two atoms will be $\frac{a\sqrt{3}}{2}$



(a) **Relationship between edge length 'a' and atomic radius 'r':**



In BCC, along cube diagonal all atoms touch each other and the length of cube diagonal is $\sqrt{3a}$.

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

i.e.
$$r = \frac{\sqrt{3a}}{4}$$

(b) **Number of atoms present in unit cell:**

$$(\frac{1}{8} \times 8) + (1 \times 1) = 1 + 1 = 2 \text{ atom or ion/unit cell.}$$

(Corner) (Body centre)

In this scenario, there is one atom or ion situated at each corner of the cube. Consequently, the contribution from the eight corners is calculated as $(\frac{1}{8\times 8})$=1, whereas the contribution from the body center is 1 within the unit cell.

Hence total number of atoms per unit cell is 1 + 1 = 2 atoms (or ions)

(c) **Packing efficiency:**

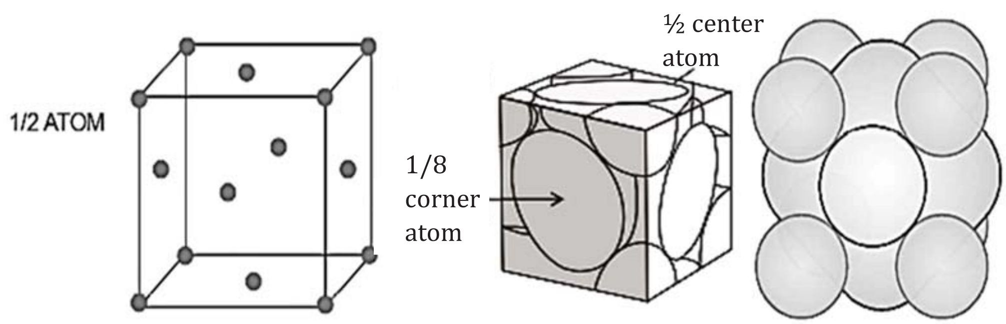
$$\text{P.E.} = \frac{n\times\frac{4}{3}\pi r^3}{V} = \frac{2\times\frac{4}{3}\times\pi\left(\frac{\sqrt{3}a}{4}\right)^3}{a^3} = \frac{\sqrt{3}\pi}{8} = 0.68 \; [\because n = 2, r = \frac{\sqrt{3}a}{4}, V = a^3]$$

In B.C.C. 68% of total volume is occupied by atom or ions.

Face Centred Cubic (F.C.C.) Cell:

A face-cantered unit cell is characterized by lattice points at each face centre in addition to lattice points at every corner. In this configuration, there are eight atoms positioned at the eight corners of the unit cell, and six atoms located at the centre of six faces. If we consider an atom at the face centre as the origin, it becomes evident that this face is shared by two adjacent cubes. Surrounding this face, there are twelve points situated at a distance equal to half the face diagonal of the unit cell.

Thus, the co-ordination number will be twelve and the distance between the two nearest atoms will be $\frac{a}{\sqrt{2}}$.



(a) **Relationship between edge length 'a' and atomic radius 'r':**

In FCC, along the face diagonal all atoms touch each other and the length of face diagonal is $\sqrt{2}a$

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

i.e. $r = \frac{\sqrt{2}a}{4} = \frac{a}{2\sqrt{2}} \quad r = \frac{a}{2\sqrt{2}}$

(b) **Number of atoms per unit cell:**

$$\left(\frac{1}{8}\times 8\right) + \left(6\times\frac{1}{2}\right) = 1 + 3 = 4 \text{ atoms/unit cell}$$

Corner faces

In this scenario, there is one atom or ion situated at each corner of the cube, and one atom or ion positioned at the centre of each face of the cube. It is noteworthy that only half of each face sphere is contained within the unit cell, and there are six such faces. The cumulative contribution of the eight corners is calculated as $(\frac{1}{8}\times 8) = 1$, while the contribution of the six face-cantered atoms is $(\frac{1}{2}\times 6)=3$ within the unit cell. Consequently, the total number of atoms per unit cell is $1 + 3 = 4$ atoms (or ions).

(c) **Packing efficiency:**

$$\text{P.E.} = \frac{n\times\frac{4}{3}\pi r^3}{V} \quad [\because \text{for FCC } n = 4, r = \frac{a}{2\sqrt{2}}, V = a^3]$$

$$\frac{4\times\frac{4}{3}\pi\times\left(\frac{a}{2\sqrt{2}}\right)^3}{a^3} = \frac{\pi}{3\sqrt{2}} = 0.74 \text{ or } 74\%$$

i.e., In FCC, 74% of total volume is occupied by atoms.

End Centered Unit Cell:

A unit cell characterized by lattice points at the centers of only one set of opposite faces, in addition to lattice points at every corner, is referred to as an end-centered unit cell.

Note: This type of Bravais lattice is obtained only in orthorhombic and monoclinic type unit cell.

Number of atoms per unit cell in cubic close packed structure of atoms

Unit Cell	Number of atoms at			No. of atoms per unit cell	Volume occupied by particles (%)
	Corners	Centres	Faces		
Simple cube	$8 \times \frac{1}{8} = 1$	0	0	1	52.4
Body Centred cube (BCC)	$8 \times \frac{1}{8} = 1$	1	0	2	68
Face Centred cube (FCC)	$8 \times \frac{1}{8} = 1$	0	$6 \times \frac{1}{2} = 3$	4	74

Ex. The lattice parameters of a given crystal are a = 5.62 Å, b = 7.41 Å and c = 9.48 Å. The three coordinate axes are mutually perpendicular to each other. The crystal is:

(A) Tetragonal (B) orthorhombic
(C) monoclinic (D) trigonal

Ans. (B)

Ex. Tetragonal crystal system has the following unit cell dimensions:

(A) $a = b = c$ and $\alpha = \beta = \gamma = 90°$ (B) $a = b \neq c$ and $\alpha = \beta = \gamma = 90°$
(C) $a \neq b \neq c$ and $\alpha = \beta = \gamma = 90°$ (D) $a = b \neq c$ and $\alpha = \beta = 90°, \gamma = 120°$

Ans. (B)

Sol. $a \neq b \neq c$ & $\alpha = \beta = \gamma = 90°$ the crystal system is orthorhombic.

Ex. In a face cantered cubic arrangement of A and B atoms whose A atoms are at the corner of the unit cell and B atoms at the face centres. One of the A atoms Is missing from one corner in unit cell. The simplest formula of the compound is

(A) A_7B_3 (B) AB_3
(C) A_7B_{24} (D) A_2B_3

Ans. (C)

Sol. $A = 7 \times \frac{1}{8} = \frac{7}{8}$; $B = 6 \times \frac{1}{2} = 3$

formula = $A7/\ 8\ B_3$ or A_7B_{24}

Ex. A compound has cubical unit cell in which X atom are present at 6 corner, Y atom are at remaining corner & only at those face centres which are not opposite to each other & Z atoms are present at remaining face canter & body canter then find.

Formula of compound (ii) Density if edge length = 2 Å.

Given: Atomic mass of X = 40 amu, Y = 60 amu, Z = 80 amu.

Sol. (i) $X = \frac{1}{8} \times 6 = \frac{3}{4}$,

$$Y = \frac{1}{8} \times 2 + \frac{1}{2} \times 3 = \frac{7}{4}$$

$$Z = \frac{1}{2} \times 3 + 1 + 1 = \frac{5}{2} = \frac{10}{4}$$

For formula: $X_{\frac{3}{4}}\ Y_{\frac{7}{4}}\ Z_{\frac{10}{4}} = X_3Y_7Z_{10}$

(ii) 1 amu = 1.67×10^{-24} gram

$$1 \text{ amu} = \frac{1}{6.02 \times 10^{24}} \text{ gram.}$$

Density $= \frac{\text{Mass}}{\text{Volume}} = \frac{\frac{3}{4}\times 40+\frac{7}{4}\times 60 \quad \frac{10}{4}\times 80}{(2\times 10^{-8})^3}$ amu/cc $= \frac{335\times 1.67\times 10^{-24}}{8\times 10^{-24}}$ = 69.8 gram/cc.