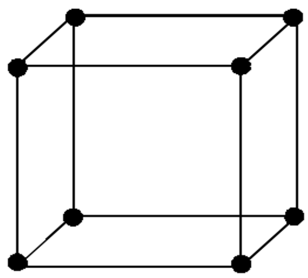
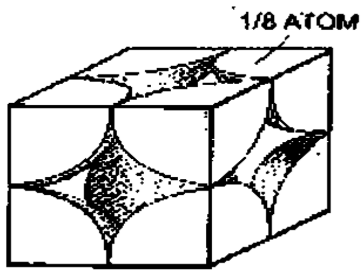
THE SOLID STATE

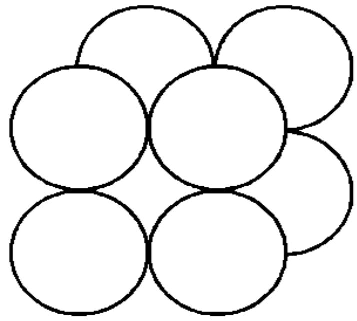
NUMBER OF ATOMS IN A UNIT CELL

SIMPLE/PRIMITIVE/BASIC UNIT CELL: -

A unit cell having lattice point only at corners called as primitive or simple unit cell. i.e. 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 centre, it will be found that this atom is surrounded by six equidistant neighbours (atoms) and thus the co-ordination number will be six. If 'a' is the side of the unit cell, then the distance between the nearest neighbours shall be equal to 'a'



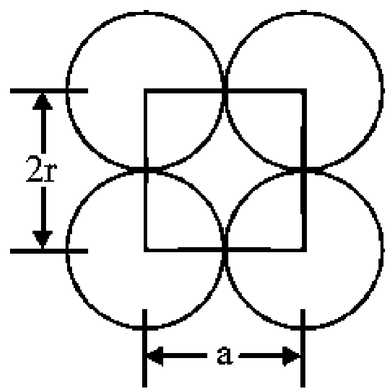




(a) Relationship between edge length 'a' and atomic radius 'r' :

$a = 2r$

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.) :

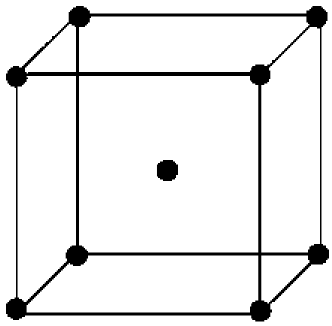
P.E. = $\dfrac{\text{Volume occupied by atoms present in unit cell}}{\text{Volume of unit cell}} = \dfrac{n \times \frac{4}{3}\pi r^3}{V}$ $\left[\because \text{Volume of atom} = \frac{4}{3}\pi r^3\right]$

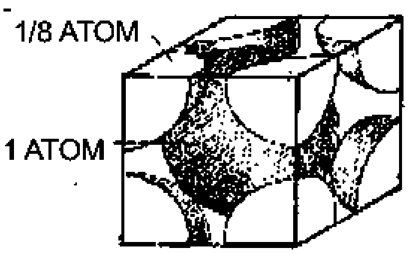
For SCC $\text{P.E.} = \dfrac{1 \times \frac{4}{3} \times \pi \times \left(\frac{a}{2}\right)^3}{a^3}$ $\left[\because r = \frac{a}{2} \text{ and } V = a^3, n = 1\right]$

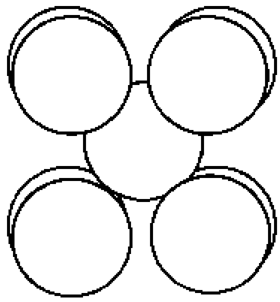
$= \dfrac{\pi}{6} = 0.524$ or $52.4\ \%$

BODY CENTRED CUBIC (B.C.C.) CELL:

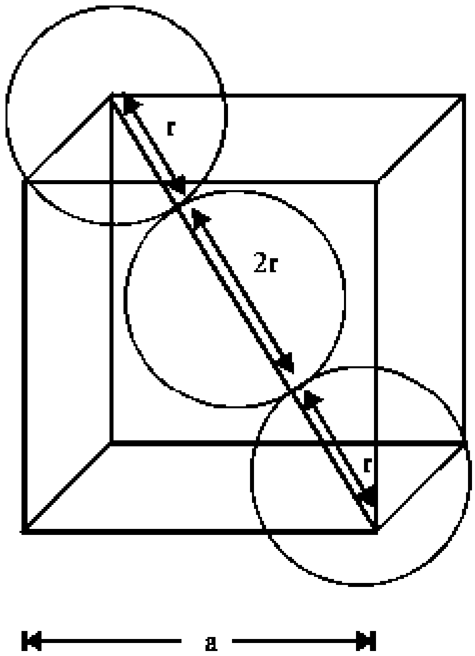
A unit cell having lattice point at the body centre in addition to the lattice point at every corner is called as body cantered unit cell. Here the central atom is surrounded by eight equidistant atoms and hence the co-ordination number is eight. The nearest distance between two atoms will be $\frac{a\sqrt{3}}{2}$







(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 atom present in unit cell:

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

(Corner) (Body centre)

In this case one atom or ion lies at each corner of the cube. Thus, contribution of the 8 corners is $\left(\frac{1}{8} \times 8\right) = 1$, while that of the body centred is 1 in the unit cell.

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

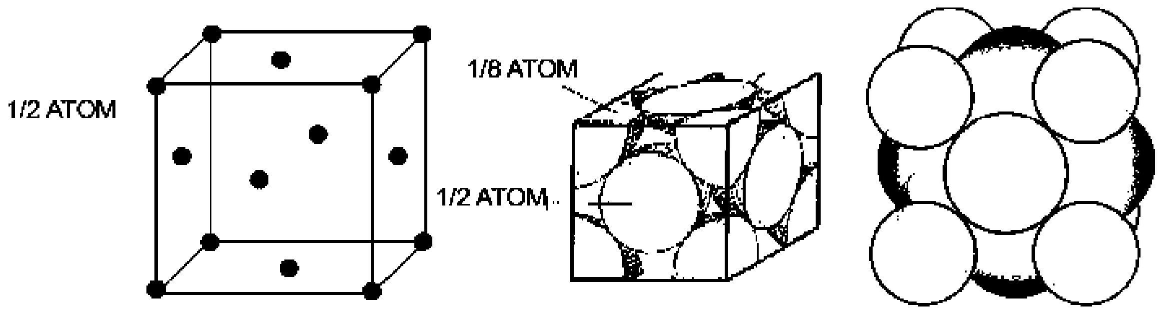
(c) Packing efficiency:

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

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

FACE CENTRED CUBIC (F.C.C.) CELL:

A unit cell having lattice point at every face centre in addition to the lattice point at every corner called as face centred unit cell. i.e., in this case there are eight atoms at the eight corners of the unit cell and six atoms at the centre of six faces. Considering an atom at the face centre as origin, it will be found that this face is common to two cubes and there are twelve points surrounding it situated at a distance which is 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. $r = \frac{\sqrt{2}a}{4} = \frac{a}{2\sqrt{2}}$ $r = \frac{a}{2\sqrt{2}}$

(b) Number of atoms per unit cell :

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

Corner faces

In this case one atom or ion lies at each corner of the cube and one atom or ion lies at the centre of each face of the cube. It may note that only $\frac{1}{2}$ of each face sphere lie within the unit cell and there are six such faces. The total contribution of 8 corners is $\left(\frac{1}{8}\times 8\right)=1$, while that of 6 face centred atoms is $\left(\frac{1}{2}\times 6\right)=3$ in the unit cell. Hence total number of atoms per unit cell is $1+3$ = 4 atoms (or ions).

(c) Packing efficiency:

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

<u>4. END CENTERED UNIT CELL</u>:

A unit cell having lattice point at the centres of only one set of opposite faces in addition to the lattice point at every corner called as end cantered 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) $1\text{ amu} = 1.67 \times 10^{-24}$ gram

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

$$\text{Density} = \frac{\text{Mass}}{\text{Volume}} = \frac{\frac{3}{4}\times40+\frac{7}{4}\times60+\frac{10}{4}\times80}{(2\times10^{-8})^3}\text{ amu/cc} = \frac{335\times1.67\times10^{-24}}{8\times10^{-24}} = 69.8\text{ gram/cc.}$$