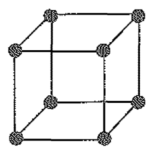
- **Number of atoms per unit cell :** A crystal lattice is made up of large number of unit cells and in different types of unit cells, particles may be present at body centre, at corners or at face centres. Most of these atoms are shared by the neighbouring unit cells because every unit is adjacent to other unit cell. Thus, only some portion of each atom belongs to a particular unit cell.

  The contribution of each atom to the unit cell :

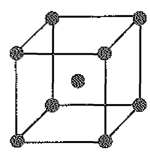
  At corners = $\frac{1}{8}$; at the face centre = $\frac{1}{2}$, body centre = 1

  - **Simple cubic unit cell :** Atoms are present at all corners of the cube. So, number of atoms per unit cell $= 8 \times \frac{1}{8} = 1$ atom.



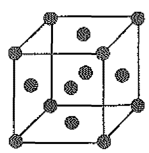
Simple cubic unit cell

  - **Body centered cubic (*bcc*) unit cell :** Atoms are present at all the corners and at the body centre. Number of atoms per unit cell $= 8 \times \frac{1}{8} + 1 \times 1 = 2$



bcc unit cell

  - **Face centered cubic (*fcc*) unit cell :** Atoms are present at the corners and at the centres of all six faces. Number of atoms per unit cell $= 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$



fcc unit cell

- The relationship between the nearest neighbour distance and radius of atom (for crystals of pure elements) and the edge of unit cell (a) is

Unit cell	Distance between nearest neighbours (d)	Radius (r)
Simple cubic	a	$\frac{a}{2}$
Face centred cubic	$\frac{a}{\sqrt{2}}$	$\frac{a}{2\sqrt{2}}$
Body centred cubic	$\frac{\sqrt{3}}{2}a$	$\frac{\sqrt{3}}{4}a$

Illustration 1

If three elements P, Q and R crystallise in a cubic solid lattice with P atoms at the corners, Q atoms at the cube centres and R atoms at the centre of the edges, then write the formula of the compound.

Soln.: As P atoms are present at the 8 corners of the cube. Therefore,

No. of P atoms in the unit cell $= 8 \times \frac{1}{8} = 1$

Q atoms are present at the cube centres,

No. of Q atoms in the unit cell = 1

R atoms are present at the edges. Since there are 12 edges and atom at each edge is shared by four atoms. Therefore,

No. of R atoms in the unit cell $= 12 \times \frac{1}{4} = 3$

$\therefore$ The formula of the compound $= PQR_3$

Density of Unit Cell

Consider a unit cell of edge 'a' (cm)

The length of the edge of the cell = a cm

Volume of unit cell = a^3 cm^3

$$\text{Density of unit cell} = \frac{\text{Mass of unit cell}}{\text{Volume of unit cell}} \quad \ldots\text{(i)}$$

Mass of unit cell

= Number of atoms in a unit cell × Mass of each atom

$= Z \times m$

Mass of an atom present in unit cell,

$$m = \frac{\text{Atomic mass}}{\text{Avogadro number}} = \frac{M}{N_0}$$

$$\text{Mass of unit cell} = Z \times \frac{M}{N_0}$$

Substituting in eq. (i), we get,

$$\text{Density} = \frac{Z \times M}{a^3 \times N_0} \text{ g cm}^{-3}$$

Illustration 2

Iron crystallizes in a bcc system with a lattice parameter of 2.861 Å. Calculate the density of iron in the *bcc* system. (Given : atomic weight of Fe = 56, $N_0 = 6.023 \times 10^{23}$ mol^{-1}.)

Soln.:

$$\text{Density, } \rho = \frac{ZM}{N_0 a^3} \quad \text{For } bcc,\ Z = 2$$

$$\rho_{Fe} = \frac{2 \times 56.0}{6.023 \times 10^{23} \times (2.861 \times 10^{-8})^3} = 7.94 \text{ g cm}^{-3}$$

Illustration 3

A metal of density 7.5×10^3 kg m^{-3} has an *fcc* crystal structure with lattice parameter $a = 400$ pm. Calculate the number of unit cells present in 0.015 kg of the metal.

Soln.:

Let V_1 be the volume of the unit cell and V_2 that of the metal sample. Given, $V_1 = (400 \times 10^{-12}\text{ m})^3 = 64 \times 10^{-30}$ m^3

$$V_2 = \frac{\text{mass}}{\text{density}} = \frac{0.015}{7.5 \times 10^3} = 2 \times 10^{-6} \text{ m}^3,$$

$$\therefore \text{ Number of unit cells} = \frac{2 \times 10^{-6}}{64 \times 10^{-30}} = 3.125 \times 10^{22}$$

PACKING IN SOLIDS

Close Packing of Spheres

- Atoms are space filling entities and structures can be described as resulting from the packing of spheres. The most efficient closest packing, can be achieved in two ways, one of which is called hexagonal close packing (*hcp*) and the other, cubic close packing (*ccp* or *fcc*).