Properties of the Unitcell (Cubic)

1. Volume of a unit cell:

The general expression for finding the volume a unit cell is

$V \quad abc\ 1 \cos^2 \quad \cos^2 \quad \cos^2 \quad 2\cos \ \cos \ \cos \ ^2 \quad ^{\frac{1}{2}}$

Where a,b,c, , and are called lattice parameters. For cubic system a=b=c and = = =90^0.

Therefore V= a^3.

2. Co-ordination number:

It is the number of nearest neighbors directly surrounding a given atom well within a crystal.

The co-ordination number for an atom in simple cubic structure is = 6

The co-ordination number for an atom in body centered cubic structure is =8

The co-ordination number for an atom in face centered cubic structure is =12

3. Number of atoms per unit cell:

In a unit cell atoms are at the corners, at the center of the faces and at the center of the body.

An atom situated at the corner share 1/8^{th} part to a unit cell.

An atom situated at the face share 1/2 part to a unit cell.

An atom situated at the center of the body share one full part to a unit cell.

1. In a simple cubic structure there are 8 corner atoms.
   ∴ Total share of all the corner atoms/unit cell = (1/8)×8 =1
   ∴ The number of atoms/unit cell in simple cube = 1
2. In a body centered cubic structure there are 8 corner atoms and an atom at the center of the unit cell.
   ∴ Total share of all the corner atoms per unit cell = (1/8)×8 = 1
   The share of an atom at the center of the body =1
   ∴ The number of atoms per unit cell in body centered cube = 1+1=2
3. In a face centered cubic structure there are 8 corner atoms and 6 face centered atoms in a unit cell.
   ∴total share of atoms at the corner/unit cell= (1/8) ×8=1
   Total share of atoms at all the faces/unit cell = (1/2) ×6=3
   ∴ The number of atoms/unit cell in face centered cube = 1+3 = 4

4. Atomic packing factor (APF)

The fraction of the space occupied by atoms in a unit cell is known as atomic packing factor. It is the ratio of the total volume occupied by the atoms in the unit cell to the total available volume of the unit cell.

1. **Simple cubic structure (SC):**

There is only one lattice point at each of the eight corners of the unit cell. In a simple cubic structure an atom is surrounded by six equidistant neighbours. Hence the co-ordination number is 6. Since each atom in the corner is shared by 8 unit cells, the total number of atoms in one unit cell is (1/8) ×8 = 1

The nearest neighbour distance '2r' is the distance between the centers of two nearest neighbouring atoms.

The nearest neighbour distance 2r = a

The number of lattice points per unit cell = 1

Volume of all the atoms in a unit cell v = $\frac{4}{3}\pi r^3$ Volume of unit cell = V = $a^3 = (2r)^3$

Packing factor is P.F = $\frac{v}{V} = \frac{\frac{4}{3}\pi r^3}{8r^3} = \frac{\pi}{6} = 0.52 = 52\%$

2. Body centered cubic structure (BCC): In a BCC structure eight atoms are present at eight corners and one atom is at the center. The co-ordination number is 8. The number of atoms per unit cell is = [(1/8)×8]+1 = 2

The lattice constant is

$(AB)^2 = a^2 + a^2 = 2a^2$

$(AC)^2 = (AB)^2 + (BC)^2$

$(4r)^2 = 2a^2 + a^2 = 3a^2$

Lattice constant $a = 4r/\sqrt{3}$

Volume of all the atoms per unit cell v = $2 \times \frac{4}{3}\pi r^3$

Volume of the unit cell $V = a^3 = \frac{64r^3}{3\sqrt{3}}$

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