Characteristic of a unit cell for cubic lattice.

The characteristic of a unit cell are
(i) Volume (ii) Atom per unit cell (iii) Co-ordination number, (iv) Atomic radius (v) Atomic packing fraction.

1. Volume of a unit cell :-

For cubic crystal $a = b = c$

∴ Volume of a unit cell $= a \times b \times c = a^3$

2. Atom per unit cell :-

The total number of atoms per unit cell is given by

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

Where N_i = No. of interior or body centred atoms.

N_f = No. of face centred atoms.

N_c = No of Corners atoms.

(i) Simple cubic crystal :- In this case

$N_i = 0$, $N_f = 0$ and $N_c = 8$

∴ Total no. of atoms $N = 0 + 0 + \frac{8}{8} = 1$

(ii) Body centred cubic crystal (BCC) :-

In this case there are 8 atoms at the eight Corners and one atom inside the cube.

∴ Total No. of atoms $N = 1 + 0 + \frac{8}{8} = 2$.

(iii) Face centred cubic crystal :-

In this case there are eight atoms at the eight Corners and one atom in each face.

i.e $N_i = 0$, $N_f = 6$, $N_c = 8$

∴ Total No of atoms $N = 0 + \frac{6}{2} + \frac{8}{8}$

$= 3 + 1 = 4$

3. Co-ordination number

The number of nearest ~~number~~ neighbours that an atom has in a unit cell is called Co-ordination number. This number can be determined as follows.

(ii) Body centred cubic crystal :- In this case there are eight atoms at the eight corners of the unit cell and one atom at the centre of the body. The central atom is surrounded by eight equidistant neighbours and hence the Co-ordination number is 8

(i) Simple cubic Crystal :- In this case for every corner atom there are six nearest neighbours (two along ± x-axis, two along ± y-axis and two along ± z-axis). Hence the Co-ordination number is Six.

(iii) Face centred cubic crystal :- In this case there are eight atoms at the eight corners of the unit cell and Six atoms at the centre of Six faces. The nearest neighbour of a corner atom is the face centred atom. Any corner atom has four face centred atoms in its own ~~above~~ plane, four in a plane above and four in a plane below it. Hence there are 12 face centred atoms for each corner atom. Thus the Co-ornination number is 12

4. Atomic radius :- see in the ~~next~~ page 15

5. Packing Fraction :-

It is defined as the ratio of volume of atoms per unit cell to the total volume of the unit cell.

$$\therefore PF = \frac{\text{NO. Of atoms in unit cell} \times \text{volume of each atom}}{\text{Volume of unit cell.}}$$

A packing factor gives us the idea as to how closely atoms are packed together in a given crystal system. A low value of PF means that the loose packing of atoms.

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and there is more unoccupied space. If PF is high, then the atoms are very closely packed in the unit cell. and there is few unoccupied space. We can calculate the value of PF in different cubic system.

(i) Simple cubic: In this case number of atoms in unit cell = 1

Atomic radius, $r = \frac{a}{2}$ where a cube edge element

∴ Volume of unit cell $= a^3$

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

∴ $PF = \frac{\pi a^3/6}{a^3} = \frac{\pi}{6} = 0.52.$

(ii) Body centred cubic (BCC): In this case

No of atoms in unit cell = 2

Atomic radius $= r = \frac{\sqrt{3}}{4}a$

Volume of one atom $= \frac{4}{3}\pi r^3 = \frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}a\right)^3 = \frac{4}{3}\pi\frac{3\sqrt{3}}{16\times 4}a^3 = \frac{\pi a^3\sqrt{3}}{16}$

∴ $PF = 2\times\frac{\pi a^3\sqrt{3}}{16a^3} = \frac{\sqrt{3}}{8} = 0.68$

(iii) Face centred cubic (FCC): In this case

No of atom in unit cell = 4

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

Volume of 4 atoms $= 4\times\frac{4}{3}\pi r^3 = 4\times\frac{4}{3}\pi\left(\frac{a}{2\sqrt{2}}\right)^3 = \frac{\pi a^3}{3\sqrt{2}}$

∴ $PF = \frac{\pi a^3}{3\sqrt{2}a^3} = \frac{\pi}{3\sqrt{2}} = 0.74$

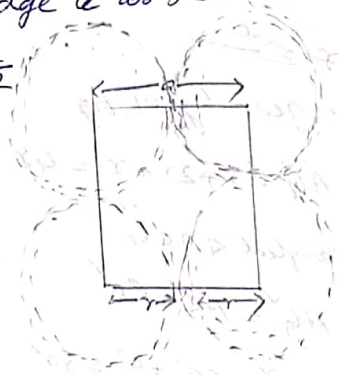
4 Atomic radius

The atoms in a crystal have same ~~fixed~~ ~~same~~ size and closely packed so as to touch each other. hence the distance between the centres of two neighbouring atoms is twice the radius of each atom. Thus the atomic radius is defined as half the distance between two nearest neighbouring atoms of same kind. It is denoted by r and is generally expressed in terms of cube edge a.

The atomic radius of cubic crystal is calculated as follows.

(i) Simple cubic system :-

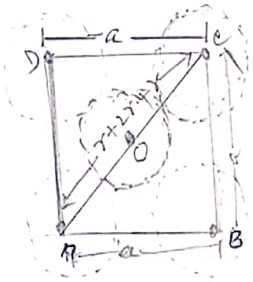
The distance between the two nearest atoms is just equal to the cube edge a as shown in the fig. Hence the atomic radius $r = \frac{a}{2}$



(ii) Face centred cubic structure :-

In this case the neighbouring atoms are a corner ~~atom~~ atom (such as A) and an atom at the centre of adjacent face (such as O) as shown in the fig. Thus the atomic radius

$r = \frac{AO}{2}$



In the right angled $\triangle ABC$

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

$$\Rightarrow (r+2r+r)^2 = a^2 + a^2$$

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

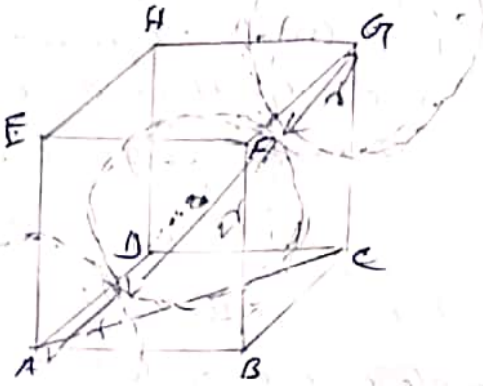
$$r^2 = \frac{a^2}{16}$$

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

(iii)

Body centred cubic structure :-

In this case the nearest neighbouring atoms are any Corner atom (such as A) and the body centre atom O. Hence the radius $r = \frac{AO}{2}$.



In the right angled $\triangle ABC$

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

$$\Rightarrow a^2 + a^2$$

$$\therefore AC = \sqrt{2}a$$

$$\Rightarrow (4r)^2 = 2a^2$$

$$\Rightarrow 16r^2 = 2a^2$$

$$r^2 = \frac{a^2}{8}$$

$$\therefore r = \frac{a}{\sqrt{8}}$$

From the geometry of fig

$$AG = r + 2r + r = 4r$$

In right angled $\triangle ACG$

$$AG^2 = AC^2 + CG^2$$

$$\text{or } (4r)^2 = 2a^2 + a^2 = 3a^2$$

$$\text{or } 16r^2 = 3a^2$$

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

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

$$= x$$