5.6 DIAMOND CUBIC STRUCTURE

Diamond is one of the allotropic forms of carbon. In diamond, carbon atoms are arranged tetrahedraly. Each carbon is attached to four other carbon atoms 1.544 A away with a C-C-C bond angle of 109.5°. Diamond structure is formed due to the combination of two interpenetrating FCC sub lattices having the origin (000) and $(a/4, a/4, a/4)$ along the body diagonal.

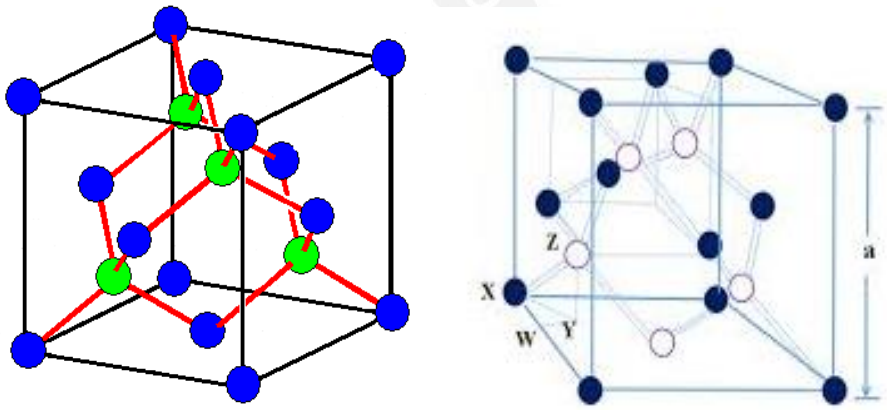


Figure:5.6.1- Diamond structure.

NUMBER OF ATOMS PER UNIT CELL

Number of atoms per unit cell in diamond carbon atoms is present at three different positions of the unit cell.

- The corner atoms represented by 'C'. There are corner atoms in the unit cell. Each corner atom is shared by 8 unit cells. The total number of corner atoms per unit cell $= 8 \times 1/8 = 1$ atom

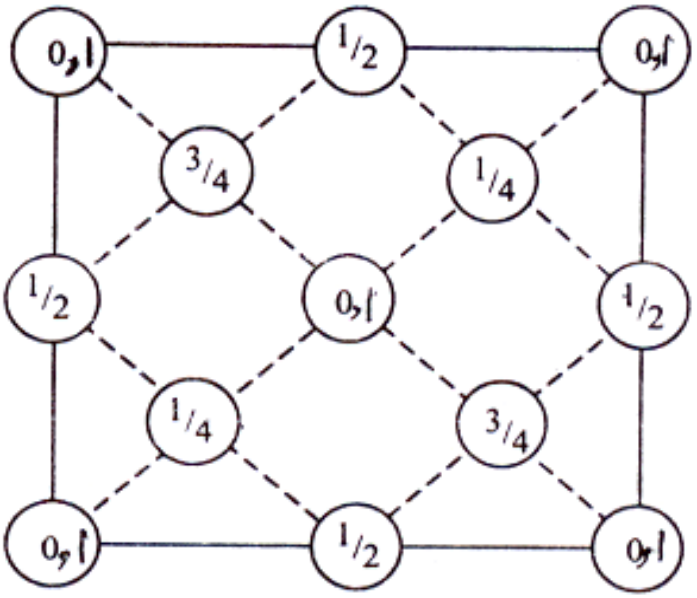


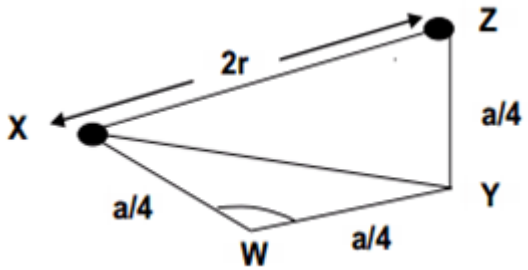
Figure:5.6.2- Diamond structure.

- Face centered atoms represented by 'F'. There are 6 face centered atoms. Each face centered atom is shared by 2 unit cells. Number of face centered atoms per unit cell= $6 \times 1/2 = 3$ atoms
- Number of atoms present inside the unit cell= 4 atoms

Total number of atoms per unit cell= 1+3+4= 8 atoms

Atomic Radius (R)

The corner atoms and face centered atoms don't touch each other. But both the corner atoms and face centered atomshave direct contact with the 4 atoms present inside the unit cell.



From fig,

$XZ^2 = XZ^2 + WY^2$

$XZ^2 = XW^2 + WY^2 + YZ^2$

$$(2r)^2 = \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2$$

$$4r^2 = \frac{3a^2}{16}$$

$$r^2 = \frac{3a^2}{4 \times 16}$$

$$\boxed{r = \frac{\sqrt{3}\,a}{8}}$$

CO-ORDINATION NUMBER

The co-ordination number is the nearest neighboring atom to a particular atom. The four atoms present inside the unit cell are the nearest neighbors for the corner atom.

The co-ordination number =4

ATOMIC PACKING FACTOR

Atomic Packing Factor (APF) = $\frac{u}{v}$..... (1)

Where,

u = Total number of atoms per unit cell X volume of one atom

v = Total volume of the unit cell Volume of an atom (spherical) is = 4/3 πr^3In diamond, we have 8 atoms per unit cell

We know that the atomic radius of diamond structure is

$$\therefore r = \frac{a\sqrt{3}}{8} \quad \text{.....(2)}$$

Volume occupied by the total number of atoms per unit cell is

$$= 8 \times \frac{4}{3}\pi r^3 \text{..... (3)}$$

since diamond has cubic structure, the volume of the unit cell is

$v = a^3$ .... (4)

Substitute equation (3) and (4) in equation (1) we get,

$$\text{APF} = \frac{8 \times \frac{4}{3}\pi r^3}{a^3}$$

$$\therefore r = \frac{a\sqrt{3}}{8}$$

$$= \frac{8 \times \frac{4}{3}\pi\left[\sqrt{3}\,a/8\right]^3}{a^3} = \frac{\pi\sqrt{3}}{16} = 0.34$$

$$APF = 34\%$$

The APF is 34%. Since the packing density is very low, it is a loosely packed structure.