Ans. (*a*) Diamond structure. A typical example of *fcc* structure is diamond. The diamond structure is of considerable importance as the basic lattice structure for many important semiconductors like Si, Ge are diamond type. In many compound semiconductors, atoms are arranged in basic diamond structure but are different on alternating sites. This is called *zinc blende lattice*.

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The diamond lattice can be supposed to be an *fcc* structure with an extra atom placed at $\frac{\vec{a}}{4} + \frac{\vec{b}}{4} + \frac{\vec{c}}{4}$ from each of the *fcc* atoms. In other words, the diamond lattice is a face centred cubic (space) lattice with primitive basis of two identical atoms at (0, 0, 0), and $\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)$ associated with each lattice point. A two dimensional view of the cell is shown in Fig. 1.27. Fractions denote height above the base in fractions of cube edge. The points 0 and 1/2 are on the *fcc* lattice. Those at 1/4 and 3/4 are on a similar lattice displaced along the body diagonal by 1/4 of its length.

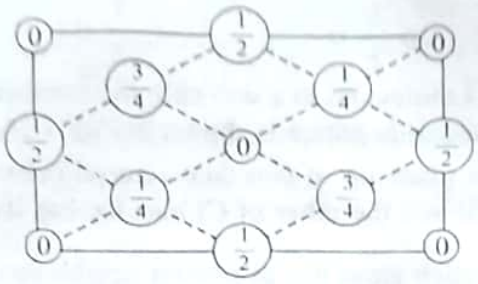

Fig 1.27

The three dimensional picture is obtained by inserting one *fcc* lattice into another *fcc* lattice displaced along the space diagonal by a quarter of its length. In the way a corner atom of one face centred cube comes in contact with a corner atom of the second cube and not with an atom in a face. Each atom of one cube may, therefore, be regarded to be at the centre of a tetrahedron formed by the four nearest neighbours belonging to the other cube. Thus each atom in a diamond structure forms *four* covalent bonds with its four nearest neighbours. The bond length is 1.544 Å and energy per bond is 3.5×10^5 Joule/mole. The crystal structure of diamond showing the tetrahedral bond arrangement is given in Fig. 1.28. Each atom has four nearest neighbours and twelve next nearest neighbours.

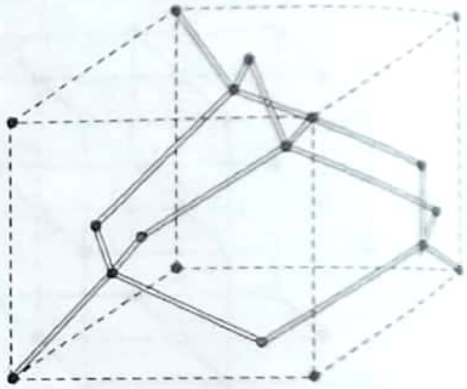
Fig 1.28

Number of nearest neighbours. The diamond structure is obtained by inserting one *fcc* lattice into another *fcc* lattice displaced along the space diagonal by a quarter of its length. Therefore, each atom has 4 *nearest neighbours* and 12 *next nearest neighbours*.

Therefore, the *co-ordination number* of each carbon atom is 4 and the *nearest neighbour distance is* $\frac{\sqrt{3}a}{4}$.

Number of atoms per unit cell. There are eight atoms per unit cell — 4 inside, 3 in the faces and one at the corners.

Packing fraction. As stated above, each atom of diamond crystal has four nearest neighbours *i.e.*, the coordination number is 4. There are eight atoms per unit cell — 4 inside, 3 in the faces and one at the corners. The body diagonal is equal to 8 r as there are 3 full spheres and 2 half spheres in it. If a is the side of the cube, then

$$(8r)^2 = 3a^2$$

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

$\therefore$ Volume occupied by the atoms in the unit cell

$$= 8 \times \frac{4}{3}\pi r^3 = 8 \times \frac{4}{3}\pi \frac{3\sqrt{3}}{8^3}a^3 = \frac{\sqrt{3}}{16}\pi a^3$$

Volume of unit cell $= a^3$

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f = Volume occupied by the atoms in the unit cell / Volume of a unit cell

$$\therefore \text{ Packing fraction } \quad f = \frac{\frac{\sqrt{3}}{16}\pi a^3}{a^3} = \frac{\sqrt{3}}{16}\pi = 34\%$$

Thus we find that packing in diamond structure is rather loose.

(*b*) Distance between the two atoms = nearest neighbour distance = $\frac{\sqrt{3}}{4}a$

Here, $a = 5\text{Å}$

$$\therefore \text{ Distance between the two atoms} = \frac{\sqrt{3}}{4} \times 5\text{Å} = \frac{1.732 \times 5}{4} = 2.16\text{Å}$$

Q. 1.15 How many atoms are there in the primitive cell of diamond? What is the length of a primitive translation vector if the cube edge $\vec{a}$ = 3.56 Å. ***(Luck. U. 1994)***

Ans. Diamond has *fcc* Bravais lattice with two carbon atoms in a primitive cell. The number of atoms in a conventional cube is 8.

If $\vec{a}$ = cube edge, then

$$\text{Primitive translation vector} = \frac{a}{\sqrt{2}} = \frac{3.56}{1.41} = 2.52 \text{ Å}$$

Q. 1.16 (*a*) Explain the

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