Lecture -6-

2-1 Simple crystal structure

2-1-1 Sodium chloride structure (NaCl)

NaClstructure is shown in Fig.12

•The lattice is FCC

•The basis is consists of 1Na^+ ion and 1Cl^- ionseparated by ½ the diagonal of a unit cube.

•There are 4 units in each unit cube.

• The coordination number of NaClis 6

•The coordinates of atoms in unit cube are

0,0,0 ;½,½,0; ½,0,½; 0, ½,½

½,½,½ ; 0,0, ½ ; 0, ½,0 ; ½,0,0

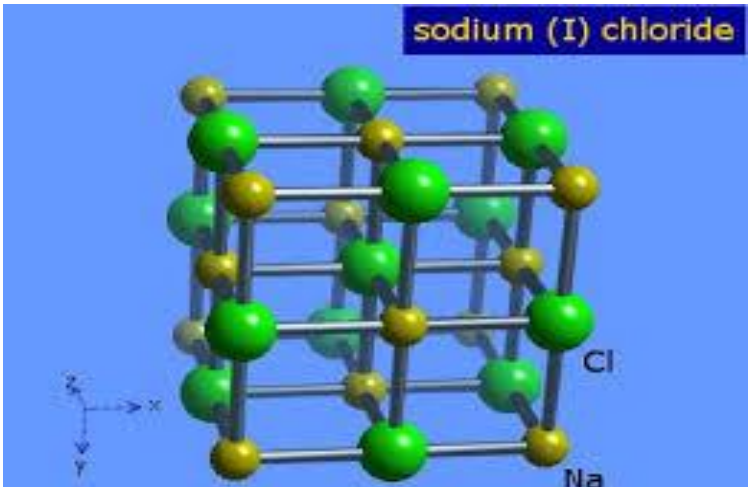


Fig.12 NaCl structure

2-1-2Cesium chloride structure(CsCl)

ClCs structure is shown in Fig.13

•The lattice is BCC

• The basis has 1 Cs^+ ion at 0,0,0 and 1 Cl^- ion at ½,½,½

• The coordination number of CsCl is8

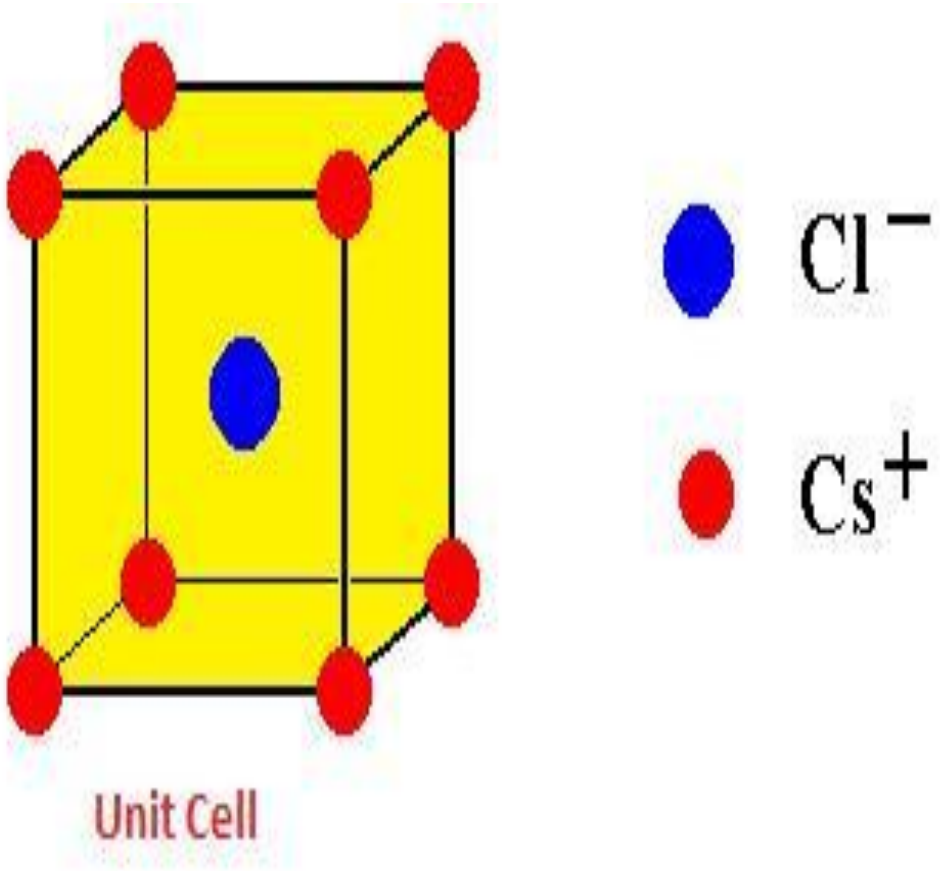


Fig.13 CsCl structure

2-1-3 Hexagonal close packed structure (hcp)

A close packed- layer of spheres (atoms) is shown in Fig. 14, with centers at points (A). A second layer goes in over (B). A third layer (C) may be added in two ways: if it goes in over (A) the order is AB ABAB and the structure is hcp (see Fig. 15).

Note:

The indices of the plane in hexagonal structure marked by (hkil), were i=-(h+k)

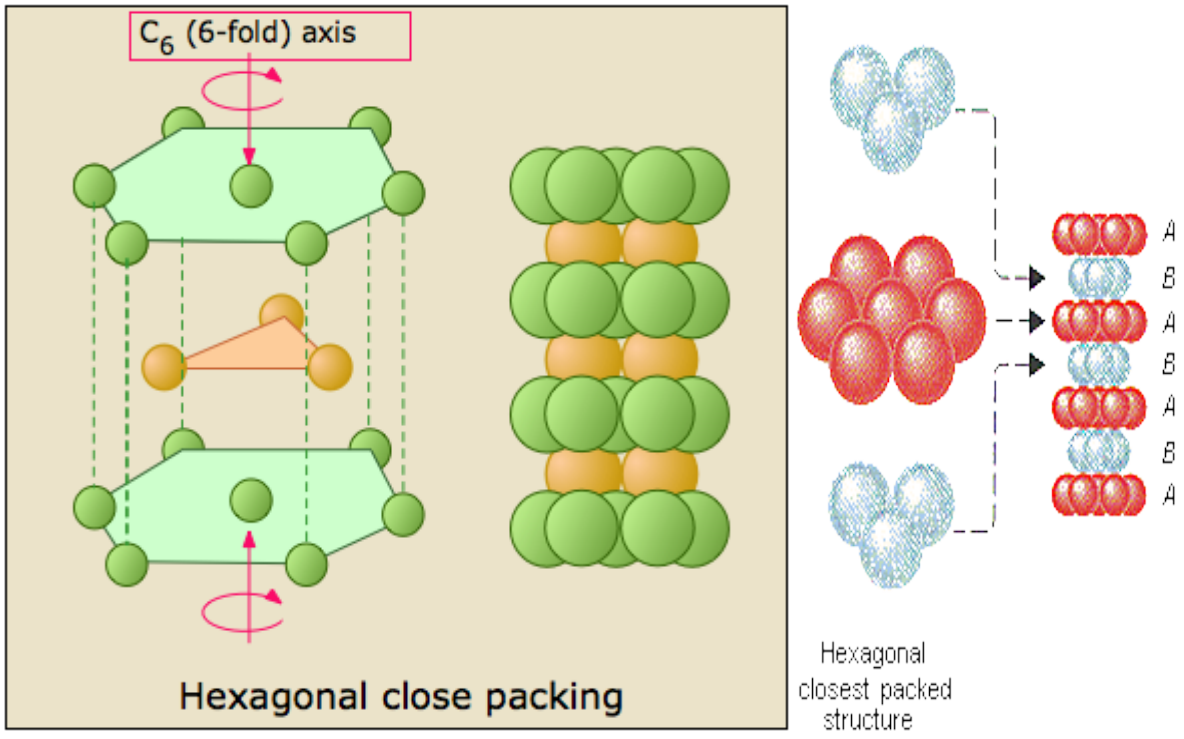
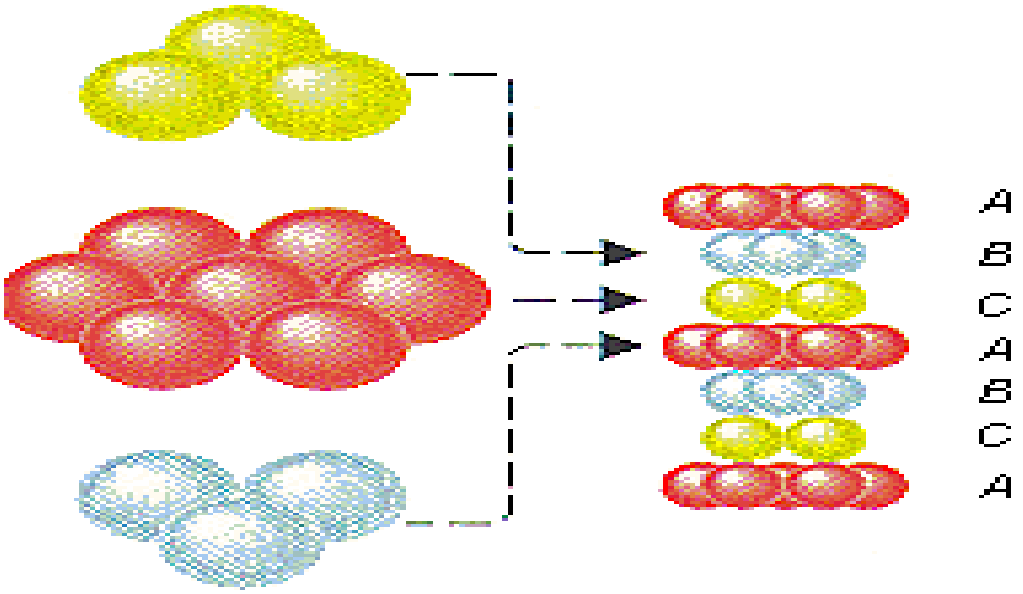


Fig.14

If it goes in over (C) the order is ABC ABC ABC and the structure is FCC.



Cubic
closest packed

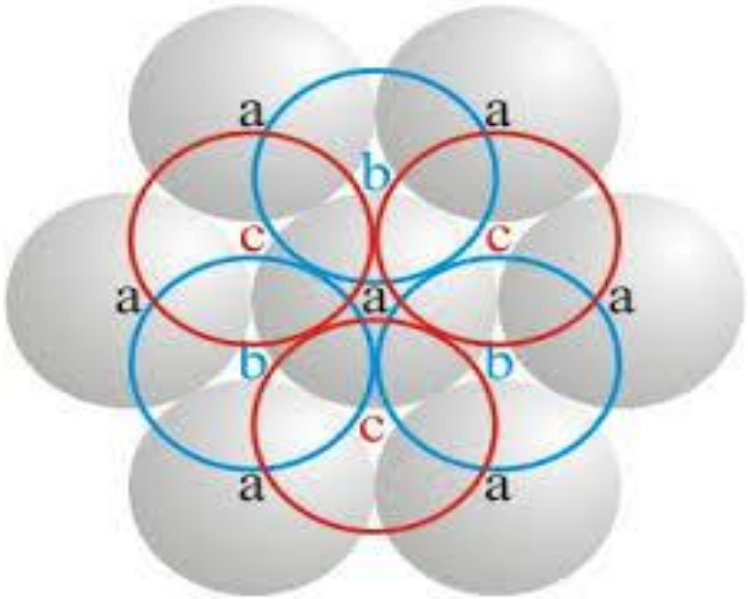


Fig. 15

2-1-4 Diamond structure

Diamond structure is shown in Fig.16

•The lattice is FCC

•The basis has 2 identical atoms at coordinateso,o,o and ¼,¼,¼.

•The coordinates of atoms in unit cube are

0,0,0 ; ½,½,0; ½,0,½; 0, ½,½

$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$; $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$; $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$; $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$

• The coordination number is 4

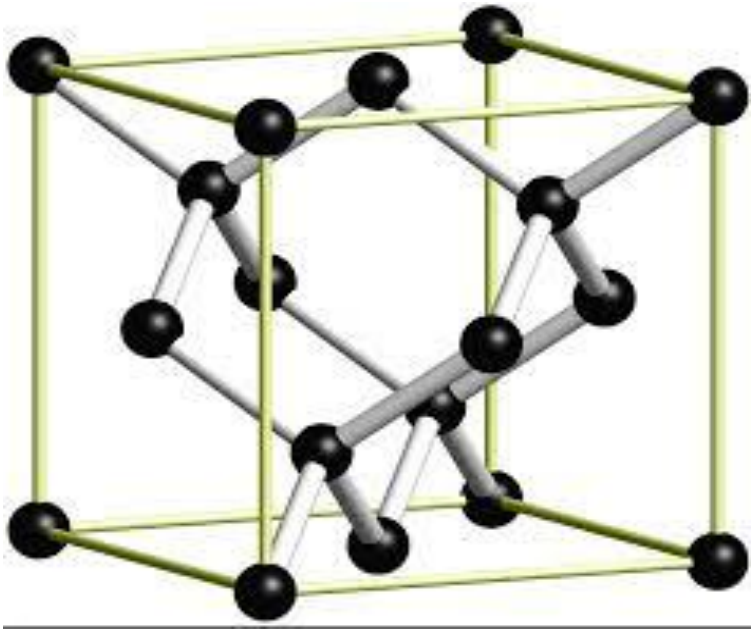


Fig.16Diamond structure

1-12 Filling factor(or packing fraction)

Filling factor = space occupied by the atoms x number of atomsper unit cell/ total volume

1. For SC

Filling factor $=\frac{4}{3}\pi r^3$X1 / $a^3=\frac{4}{3}\pi(\frac{a}{2})^3$X1 / a^3=52%

2. For BCC

Filling factor$=\frac{4}{3}\pi r^3$X2 / $a^3=\frac{4}{3}\pi(\sqrt{3}a/4)^3$X2 / a^3=68%

3. ForFCC

Filling factor $=\frac{4}{3}\pi r^3$X4 / $a^3=\frac{4}{3}\pi(\frac{a}{2\sqrt{2}})^3$X4 / a^3=74%

4. For Diamond structure

Filling factor $=\frac{4}{3}\pi r^3$X8/ $a^3=\frac{4}{3}\pi(\sqrt{3}\frac{a}{8})^3$X1 / a^3=34%