The Crystal Structure of Potassium Chloride

The diffraction pattern of KCI in powdered crystal method proves primitive cubic lattice for KCl. But KCl is isomorphous with NaCl having same crystal structure like NaCl i.e. KCl must have fcc structure. Inspite of having f.c.c. structure the diffraction pattern indicates simple cubic structure for to the fact that K^+ and Cl^- ions are isoelectronic and have the same diffracting power. So, X-ray diffraction cannot distinguish between K^+ and Cl^-. Hence all the ions in the f.c.c. unit cell of KCl are equivalent to X-ray. Therefore the f.c.c unit cell structure is equivalent to the combination of eight simple cubes where K^+ and Cl^- ions occupy alternate corners of the cube and behave in the same manner towards diffraction. This is why diffraction pattern indicates simple cubic structure for KCl.

Except caesium halides, all the other alkali metal halides have interpenetrating face-centred cubic structure. Like KCI, RbBr has a simple cubic structure as Rb^+ ion and Br^- ions are isoelectronic and tave same diffracting power.

Packing in cubic crystal structure and void-space

Simple cubic structure (or primitive cubic cell): In this structure atoms occupy only the corner positions and they are in contact with one another. Thus each comer atom is equally shared by adjacent eight such unit cubes.

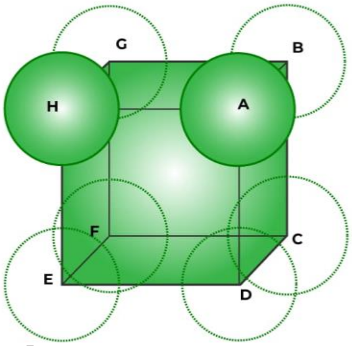

Fig26: Packing in simple cube

Hence each corner atom contributes 1/8th to each cube. Hence the number of atoms associated with a unit cell = 8x1/8=1. i.e, effectively 1 atom is present per unit cell.

If r be the radius of the atom, vol. of the atom = $\frac{4}{3}\pi r^3$

Side length(a)of cube = 2r

Vol. of unit cell = $a^3 = (2r)^3 = 8r^3$

% of space occupied by atoms = $\dfrac{\frac{4}{3}\pi r^3}{8r^3}$ X100 = 52.36

i.e . 52.36% of the space of the unit cell is occupied by atoms.

(2) Face-centred cubic lattice: Solidified inert gases and several metals such Cu , Ag, Au possess f.c.c structures. In the f.c.c. lattice of an atom, atoms are present at each comer and at the face-centred position of the cube in a closest packed manner. This state is attained when atoms along the face diagonal are in contact with one another. If a be the sidelength of the cube, then the face diagonal = $\sqrt{2}a$ and face diagonal = 4r.

So $\sqrt{2}a = 4r$

or, $a = 2\sqrt{2}\,r$

volume of the unit cell= $(2\sqrt{2}\,r)^3 = 16\sqrt{2}\,r^3$

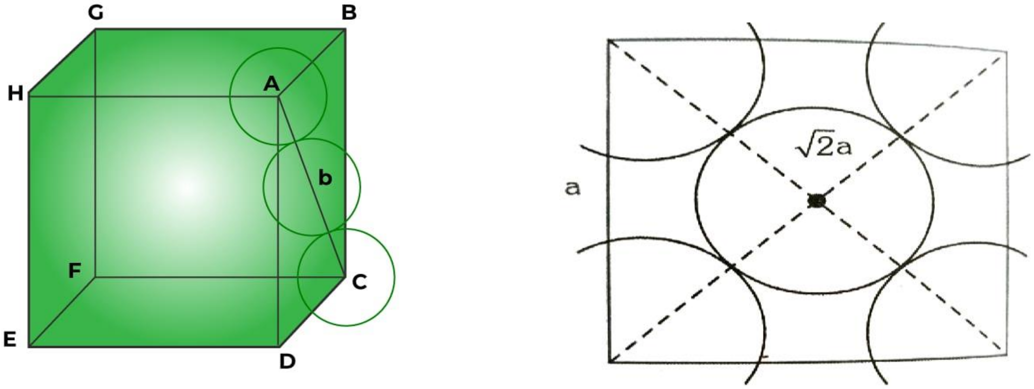

Fig. 27 :A face of f.c.c. structure

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Each comer atom is shared equally by eight adjacent corners of 8 unit cells.

8 corner atoms of the cube atom =8X1/8 atom= 1 atom per unit cell.

Each face centred atom is shared by two adjacent faces of two unit cell. So, 6 face-centred atoms of the cube =6 X ½ = 3 atoms per unit cell. Therefore, each unit cell possesses effec atoms of the cube (1+3) or, 4 atoms .

Volume of 4 atoms per unit cell=4X $\frac{4}{3}\pi r^3$

% of space occupied by atoms in a unit cell = $\frac{4X\frac{4}{3}\pi r^3\ X100}{16\sqrt{2}\,r^3}$

i.e. 74% of the space of the unit cell is occupied by matter.

(iii) Body-centred cubic structure: In this crystal lattice atoms are present at the comers and at the centre of the unit cell in a closest packed manner, i.e., the atoms are adjacent to another only along the cube diagonal. If 'a' be side-length of the cube and r be the radius the atom, then the cube diagonal = $\sqrt{3}\,a$

$$\sqrt{3}\,a\ =4r,\ \text{i,e}\ a=\frac{4}{\sqrt{3}}r$$

$$a^3=\left(\frac{4}{\sqrt{3}}r\right)^3=\frac{64}{3\sqrt{3}}r^3$$

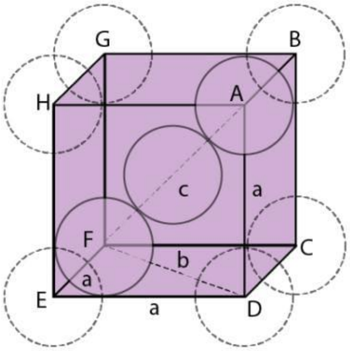

Fig 28: A face of b.c.c. structure

Fach comer of atom is equally shared by eight adjacent cubes. So per unit cell contribution of eight corner atoms = 8 X 1/8 = 1 .

The atoms present at the centre of the unit cell solely belongs to that cell. Hence effective number of atoms present per unit cell = 1+1=2.

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Volume of 2 atoms = 2 x $\frac{4}{3}\pi r^3$

% of space occupied by the atoms in unit cell

$$= \frac{\frac{8}{3}\pi r^3}{\frac{64}{3\sqrt{3}} r^3} = \frac{\sqrt{3}\pi}{8} \text{x} 100 = 68.02$$

i.e 68% space of unit cell occupied by atoms . Alkali metals have b.c.c structure. Therefore, among the cubic structure f.c.c. structure is most closely packed.

Density of Cubic Crystals

Simple cubic structures : In a simple cube, 1 atom is present per unit cell of side length =a =2r

So volume of unit cell $=a^3=(2r)^3=8r^3$

Hence density $(\rho) = \frac{A}{N_0 \, 8r^3}$

Where A is the gm atomic wt. of metal.

2. Face centred cubic: No of atoms present per unit cell =8X1/8+6X1/2=4

Along the face diagonal the atoms remain in contact with one another.

So $\sqrt{2}a = 4r$, where a= side length of the cube.

So density $(\rho) = \frac{4A}{N_0 \, a^3} = \frac{A}{16\sqrt{2}\, r^3 N_0} = \frac{A}{4\sqrt{2}\, r^3 N_0}$

3. Body Centred Cube:

No of atoms per unit cell= $8x\frac{1}{8}+1=2$

Along the cube diagonal the atom remain connected.

$$\sqrt{3}\,a = 4r \text{ or } a = \frac{4}{\sqrt{3}}r$$

$$\text{So density } (\rho) = \frac{2A}{\left(\frac{4}{\sqrt{3}}r\right)^3 N_0} = \frac{3\sqrt{3}\,A}{32r^3N_0}$$