

1. Iron exhibits *bcc* structure at room temperature. Above 900°C , it transforms to *fcc* structure. The ratio of density of iron at room temperature to that at 900°C (assuming molar mass and atomic radii of iron remains constant with temperature) is

(a) $\frac{\sqrt{3}}{\sqrt{2}}$

(c) $\frac{3\sqrt{3}}{4\sqrt{2}}$

(b) $\frac{4\sqrt{3}}{3\sqrt{2}}$

(d) $\frac{1}{2}$

bcc (Z=2) $a = \frac{4r}{\sqrt{3}}$

fcc (Z=4) $a = 2\sqrt{2}r$

(2018)

$d = \frac{ZM}{NV \sim a^3}$

11. Structure of a mixed oxide is cubic close packed (ccp). The cubic unit cell of mixed oxide is composed of oxide ions. One fourth of the tetrahedral voids are occupied by divalent metal A and the octahedral voids are occupied by a monovalent metal B . The formula of the oxide is

n Sphere
 n Ov
 $2n$ Tv

- (a) ABO_2 (b) A_2BO_2
 (c) $A_2B_3O_4$ (d) AB_2O_2 (2012)

Lattice (O^{2-})

1 O^{2-}	}
1 Ov	
2 Tv	

$$A^{2+} = \frac{1}{4} \times 2 = 2$$

$$B^+ = 1$$

$O^{2-} = 1$
$A^{2+} = 2$
$B^+ = 1$

eight half

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$AB_2O_4 \checkmark$
 $+2(+3)2 - 8 = 0$

trivalent

$(+2 (+3)2 - 4 = 0)$

1 O^{2-} $A^{2+} = \frac{1}{8} \times 2 = \frac{1}{4}$
 1 OV
 2 TV $B^{3+} = \frac{1}{2} \times 1 = \frac{1}{2}$

O^{2-} A^{2+} B^{3+}
 1 $\frac{1}{4}$ $\frac{1}{2}$



1) What % of Td is occupied by A^{2+}

2) What % of Ov is occupied by B^{3+}



$$\% \text{ occupancy} = \frac{1}{8} \times 100 = 12.5\%$$

$$\% \text{ occupancy} = \frac{2}{4} \times 100 = 50\%$$

57. Experimentally it was found that a metal oxide has formula $M_{0.98}O$. Metal M , is present as M^{2+} and M^{3+} in its oxide. Fraction of the metal which exists as M^{3+} would be

(a) 5.08%

(b) 7.01%

(c) 4.08%

(d) 6.05%

(2013)

$$M^{3+} = x, \quad M^{2+} = 0.98 - x$$

$$3x + 2(0.98 - x) = 2, \quad x =$$



$$0.98x - 2 = 0$$

$$x = \frac{200}{98} = 2.06$$

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(2013)

$$M^{3+} = x, \quad M^{2+} = 0.98 - x$$

$$3x + 2(0.98 - x) = 2, \quad x = 0.04$$

$$\underline{M_{0.98}O}$$

$$0.98x - 2 = 0$$

$$x = \frac{200}{98} = 2.06$$

$$\% M^{3+} = \frac{0.04}{0.98} \times 100$$
$$= \underline{4.08\%}$$

69. If the unit cell of a mineral has cubic close packed (ccp) array of oxygen atoms with m fraction of octahedral holes occupied by aluminium ions and n fraction of tetrahedral holes occupied by magnesium ions, m and n , respectively, are

(a) $\frac{1}{2}, \frac{1}{8}$

(b) $1, \frac{1}{4}$

(c) $\frac{1}{2}, \frac{1}{2}$

(d) $\frac{1}{4}, \frac{1}{8}$

(2015)

CCP ($Z=4$) = no of O atoms

Ov = 4 } no of $Al^{+3} = m \times 4$

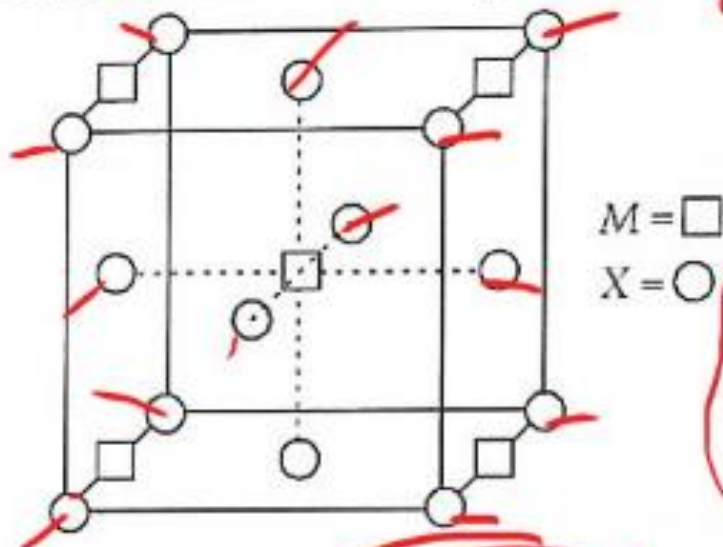
Tv = 8 } no of $Mg^{2+} = n \times 8$

Formula $Al_{4m} Mg_{8n} O_4$

$$4m(+3) + 8n(-2) + 4(-2) = 0$$

$$\underline{3m + 4n = 2}$$

71. A compound M_pX_q has cubic close packing (ccp) arrangement of X. Its unit cell structure is shown below. The empirical formula of the compound is



$$8 \times \frac{1}{8} = 1, \quad 6 \times \frac{1}{2} = 3$$

$$X = 4$$

$$\text{edge contribution} = \frac{1}{4}$$

$$\frac{4}{4} = 1$$

$$\text{Body center} = 1$$

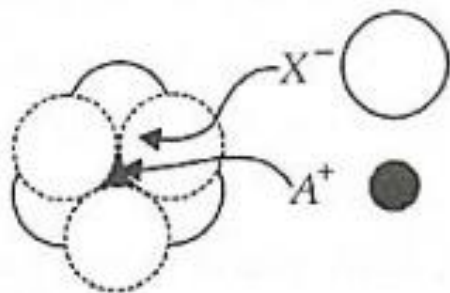
$$2$$

- (a) MX
 (c) M_2X

- (b) MX_2
 (d) M_5X_{14}

(2012)

70. The arrangement of X^- ions around A^+ ion in solid AX is given in the figure (not drawn to scale). If the radius of X^- is 250 pm, the radius of A^+ is



$$\frac{r_c}{r_a} = 0.414$$

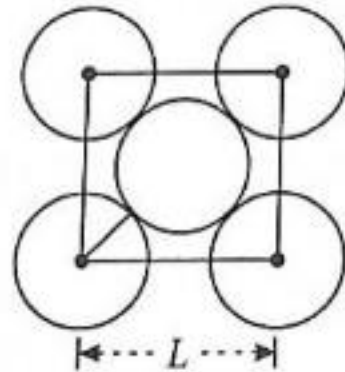
$$\frac{r_c}{250} = 0.414$$

- (a) 104 pm
 (c) 183 pm

- (b) 125 pm
 (d) 57 pm

(2013)

73. The packing efficiency of the two-dimensional square unit cell shown below is



$$\text{Packing efficiency} = \frac{\text{Area Covered}}{\text{Total area}}$$

$$\text{radius of circle} = r$$

$$\text{edge length of Sq} = a$$

(a) 39.27%

(b) 68.02%

(c) 74.05%

(d) 78.54%

(2010)

$$\text{Area covered} = \frac{2 \times \pi r^2}{a^2} = \frac{2 \pi r^2}{(2\sqrt{2}r)^2} = \frac{\pi}{4} =$$

58. Ferrous oxide has a cubic structure. The length of edge of the unit cell is 5 \AA . The density of the oxide is 4.0 g cm^{-3} . Then the number of Fe^{2+} and O^{2-} ions present in each unit cell will be

- (a) four Fe^{2+} and four O^{2-} (b) two Fe^{2+} and two O^{2-}
 (c) four Fe^{2+} and two O^{2-} (d) two Fe^{2+} and four O^{2-}

$$d = \frac{\Sigma M}{NV}$$

↘ 4 ✓

61. Number of unit cells in 4 g of X (atomic mass = 40) which crystallises in *bcc* pattern is (N_A = Avogadro number)

(a) $0.1 N_A$

(b) $2 \times 0.1 N_A$

(c) $\frac{0.1 N_A}{2}$

(d) $2 \times N_A$

40g $\longrightarrow N_A$
 4g $\longrightarrow 0.1 N_A$

2 atoms forms 1 unit cell

$0.1 N_A \longrightarrow \frac{0.1 N_A}{2}$

65. The density of a pure substance 'A' whose atoms are in cubic close packed arrangement is 1 g/cm^3 . If all the tetrahedral voids are occupied by 'B' atom, what is the density of resulting solid in g/cm^3 . [Atomic mass (A) = 30 g/mol and atomic mass (B) = 50 g/mol]
- (a) 3.33 (b) 4.33 (c) 2.33 (d) 5.33

Let volume of CCP/FCC = V

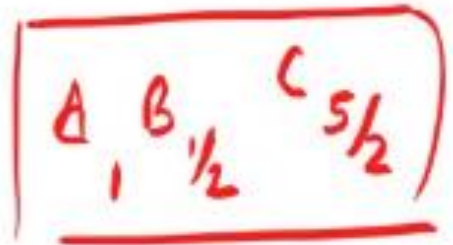
Total density = 4.33 g/cm^3

$$d_A = \frac{4 \times M_A}{N_A V} \quad \left\{ \begin{array}{l} d_A = 0.3 \\ d_B \end{array} \right.$$

$$d_B = \frac{8 \times M_B}{N_A V} \quad \left\{ \begin{array}{l} d_B = \frac{d_A}{0.3} = 3.33 \end{array} \right.$$

A compound formed by A, B and C in which A is arranged in ccp, B is present in 25% of the tetrahedral voids and C is present in all the remaining voids (tetrahedral as well as octahedral). Determine formula of compound

$$\boxed{A = 1, \quad OV = 1, \quad TV = 2}$$



$$2 \times \frac{25}{100} = B = \frac{1}{2}$$

$$OV = 1, \quad \frac{3}{2}$$

A compound is consist of A, B and C. The distribution of A, B, C in unit cell is as follows

A is at corner

B is at body centre

C is at face centre

(i) Estimate the formula.

(ii) Estimate the formula if:

- (a) all the atoms along one of the face diagonal are removed.
- (b) all the atoms along one of body diagonal are removed.
- (c) all the atoms along one of axis is removed if body centre is at origin.
- (d) all atoms along one of axis is removed if origin is at any of the corner

(ABC_3) ✓

$(A_3B_4C_0)$

a) $A_3B_4C_0$

b) AC_4

c) AC_2

d) $A_3B_4C_{12}$



7 In a crystalline solid, anions C are arranged in cubic close-packing. Cations A occupy 50% of the tetrahedral voids and cations B occupy 50% of the octahedral voids. What is the formula of the solid?

$$\begin{array}{l}
 C = 1 \\
 OV = 1 \\
 TV = 2
 \end{array}
 \left\{
 \begin{array}{l}
 2 \times \frac{50}{100} = A = 1 \\
 1 \times \frac{50}{100} = B = \frac{1}{2}
 \end{array}
 \right.$$



PROBLEM 13 Chromium metal crystallizes with a body-centred cubic lattice. The length of the unit cell edge is found to be 287 pm. Calculate the atomic radius. What would be the density of chromium in g/cm^3 ?
 (IIT July 1997)

BCC lattice $r = \frac{\sqrt{3}a}{4} = \frac{\sqrt{3} \times 287}{4} = 125$

$$d = \frac{ZM}{NU} \rightarrow 7.03 \text{ g/cm}^3$$

PROBLEM 16 A compound AB has a rock type structure with $A:B = 1:1$. The formula weight of AB is $6.023y$ amu and the closest A - B distance is $y^{1/3}$ nm.

(a) Calculate the density of lattice.

(b) If the observed density of lattice is found to be 20 kg m^{-3} , then predict the type of defect. (IIT 2004)

$$a = 2(a^+ + b^-) = \underline{2y^{1/3} \times 10^{-9} \text{ m}}$$

$$D = \frac{ZM}{NV} = \frac{4 \times y \times 10^{-3}}{6.023 \times 10^{23} \times (2y^{1/3} \times 10^{-9})^3} = 5$$