

Match the columns.

Column I	Column II
(A) Rock salt structure	(P) Coordination number of cation is 4.
(B) Zinc blend structure	(Q) $\frac{\sqrt{3}a}{4} = r^+ + r^-$
(C) Fluorite structure	(R) Coordination number of cation and anion is same.
	(S) Distance between two nearest anion is $\frac{a}{\sqrt{2}}$ .

A solid contains  $A^{n+}$  and  $B^{m-}$  ions. The structure of solid is FCC for  $B^{m-}$  ions and  $A^{n+}$  ions are present in one-fourth of the tetrahedral voids as well as in one-fourth of octahedral voids. What is the simplest formula of solid?

- (a)  $A_3B_4$       (b)  $A_4B_3$   
 (c)  $AB_2$       (d)  $A_2B$

Sodium oxide has anti-fluorite structure. The percentage of the tetrahedral voids occupied by the sodium ions is

- (a) 12%      (b) 25%  
 (c) 50%      (d) 100%

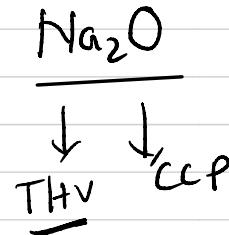
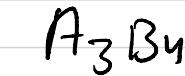
Copper has a FCC lattice with a unit cell edge length of  $\frac{0.5}{\sqrt{2}}$  nm.

Q What is the size of the largest atom that could fit into octahedral holes of the lattice without disturbing the lattice?

- (a)  $\frac{0.207}{\sqrt{2}}$  nm      (b)  $\frac{0.366}{\sqrt{2}}$  nm  
 (c) 0.092 nm       (d) 0.052 nm

$$B = 4$$

$$A = \frac{1}{4} \times 8 + \frac{1}{4} \times 4 = 3$$



$$4r_- = a\sqrt{2} = 0.5$$

$$r_- = 0.5/4$$

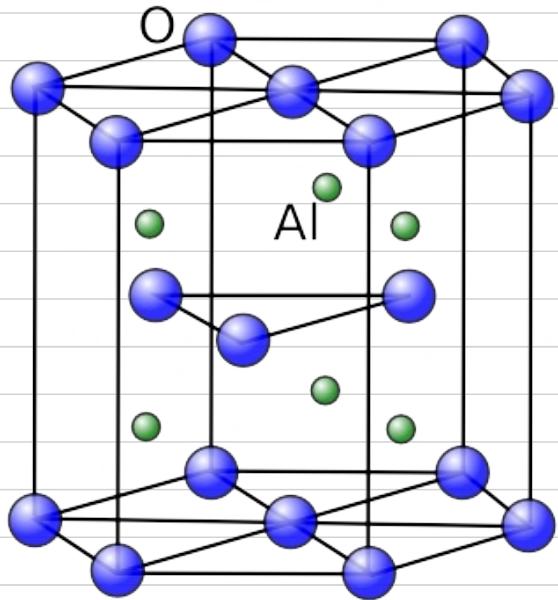
Q What is the size of the largest atom that could fit into tetrahedral holes of the lattice without disturbing the lattice?

- (a) 0.028 nm      (b) 0.052 nm  
 (c)  $\frac{0.1125}{\sqrt{2}}$  nm      (d)  $\frac{0.207}{\sqrt{2}}$  nm

$$\frac{r_+}{r_-} = 0.414 \Rightarrow r_+ = 0.414 \times \frac{0.5}{4} = 0.052$$

$$\frac{r_+}{r_-} = 0.225 \Rightarrow r_+ = 0.225 \times \frac{0.5}{4} = 0.028$$

## Corundum type (or $\text{Al}_2\text{O}_3$ ):-



$\text{O}^{2-}$  = All hcp lattice pt  
 $\text{Al}^{+3}$  =  $\frac{2}{3} \text{ of OHV}$  } info

Effective  $\text{O}^{2-}$  = 6

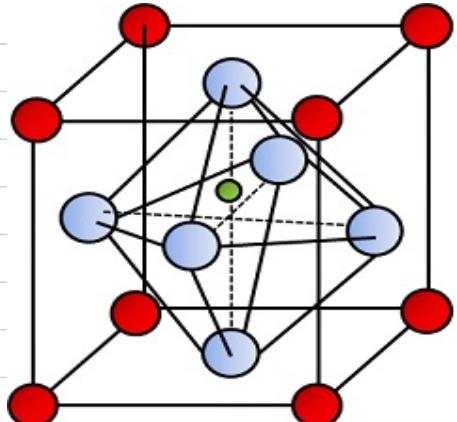
$$\text{Al}^{+3} = \frac{2}{3} \times 6 = 4$$

↓

$\text{Al}_2\text{O}_3$

CN:  $6 : 4$

## Pervoskite type ( $\text{CaTiO}_3$ ):-



$\text{Ca}^{2+}$  = All corners of cube

$\text{O}^{2-}$  = All Face centre

$\text{Ti}^{4+}$  = Body centre

$$\text{Ti}^{+4} \begin{cases} \text{O}^{2-} = 6 \\ \text{Ca}^{+2} = 8 \end{cases}$$

$$\begin{array}{c|c} \text{O}^{2-} & \begin{array}{l} \text{Ca}^{+2} = 4 \\ \text{Ti}^{+4} = 2 \end{array} \\ \hline \text{Ca}^{+2} & \begin{array}{l} \text{O}^{2-} = 12 \\ \text{Ti}^{+4} = 8 \end{array} \end{array}$$

## Spinel and Inverse Spinel :- (AB<sub>2</sub>O<sub>4</sub>) :-

### Spinel

$O^{+2} = \text{All CCP lattice Pb} = 4$

$A^{+2} = \frac{1}{8} \text{ th THV} = 1$

$B^{+3} = \frac{1}{2} \text{ OHV} = 2$

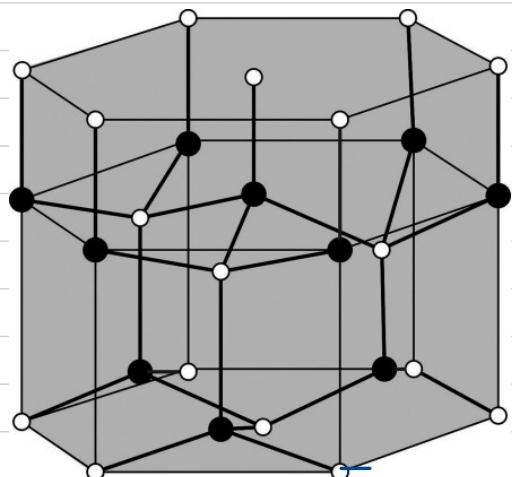
### Inverse Spinel

$O^{+2} = \text{All CCP lattice Pb} = 4$

$A^{+2} = \frac{1}{8} \text{ th THV} = 1$

$B^{+3} = \frac{1}{4} \text{ th OHV} + \frac{1}{8} \text{ th THV} = 2$

## \* Wurtzite (or ZnS) :-



$S^{-2} = \text{All HCP lattice Pt}$

$Zn^{+2} = \text{Alternate THV}$

# Defects in crystals

# formation of defect is endothermic which increase entropy

$$\Delta G_f = \underbrace{\Delta H}_{+ve} - T \cdot \Delta S_{-ve} = -ve \Rightarrow \text{Spontaneous}$$

$T \uparrow \Rightarrow \text{defect} \uparrow$

# If defect is present on a position / point in crystal then it is called point defect.

## Types of Point Defects :

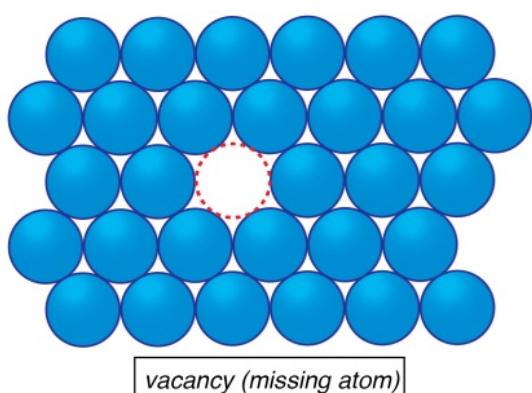
Point defect can be classified into three types:

- (i) Stoichiometric defects
- (ii) Non-stoichiometric defects
- (iii) Impurity added defect

### Stoichiometric Defect

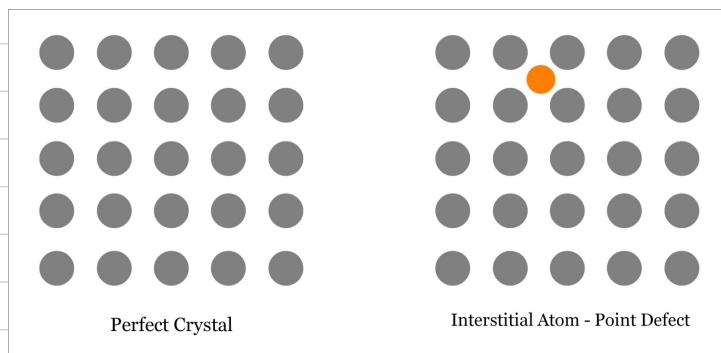
:- If due to defect stoichiometry of crystal is not affected then it is called Stoichiometric defect.

#### (a) Vacancy Defect :



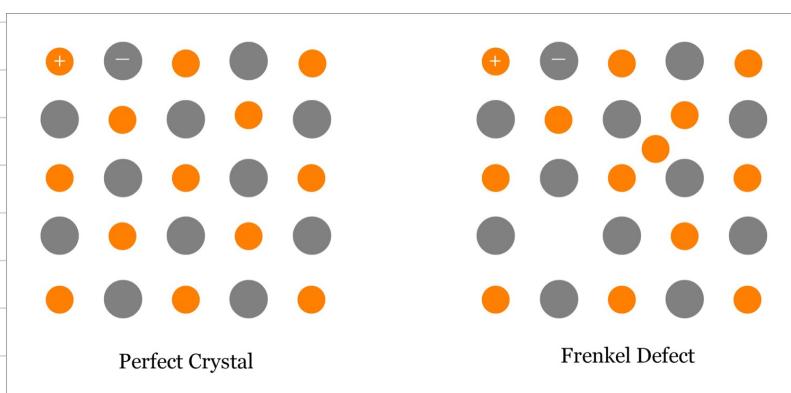
# density ↓

## (b) Interstitial Defect :



density ↑

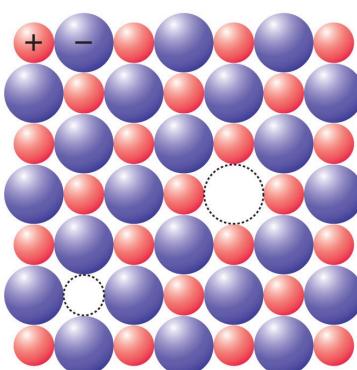
## (c) Frenkel Defect :



$\Rightarrow$  density = const  
 $\Rightarrow$  Dislocation defect.  
 $\Rightarrow$  Conduction ↑  
 $\Rightarrow$  Low coordination No compound. where diff in size of cation and anion is large  
# Dielectric constant example, ZnS, AgCl, AgBr

and AgI due to small size of  $Zn^{2+}$  and  $Ag^+$  ions.

## (d) Schottky Defect :



A<sup>+</sup>B<sup>-</sup>

# density ↓

# Conduction ↑

# Diff in size of cation and anion is not very large.  
High coordination No compound

$10^6$  Schottky pairs per  $cm^3$  at room temperature. In  $1\text{ cm}^3$  there are about  $10^{22}$  ions. Thus, there is one Schottky defect per  $10^{16}$