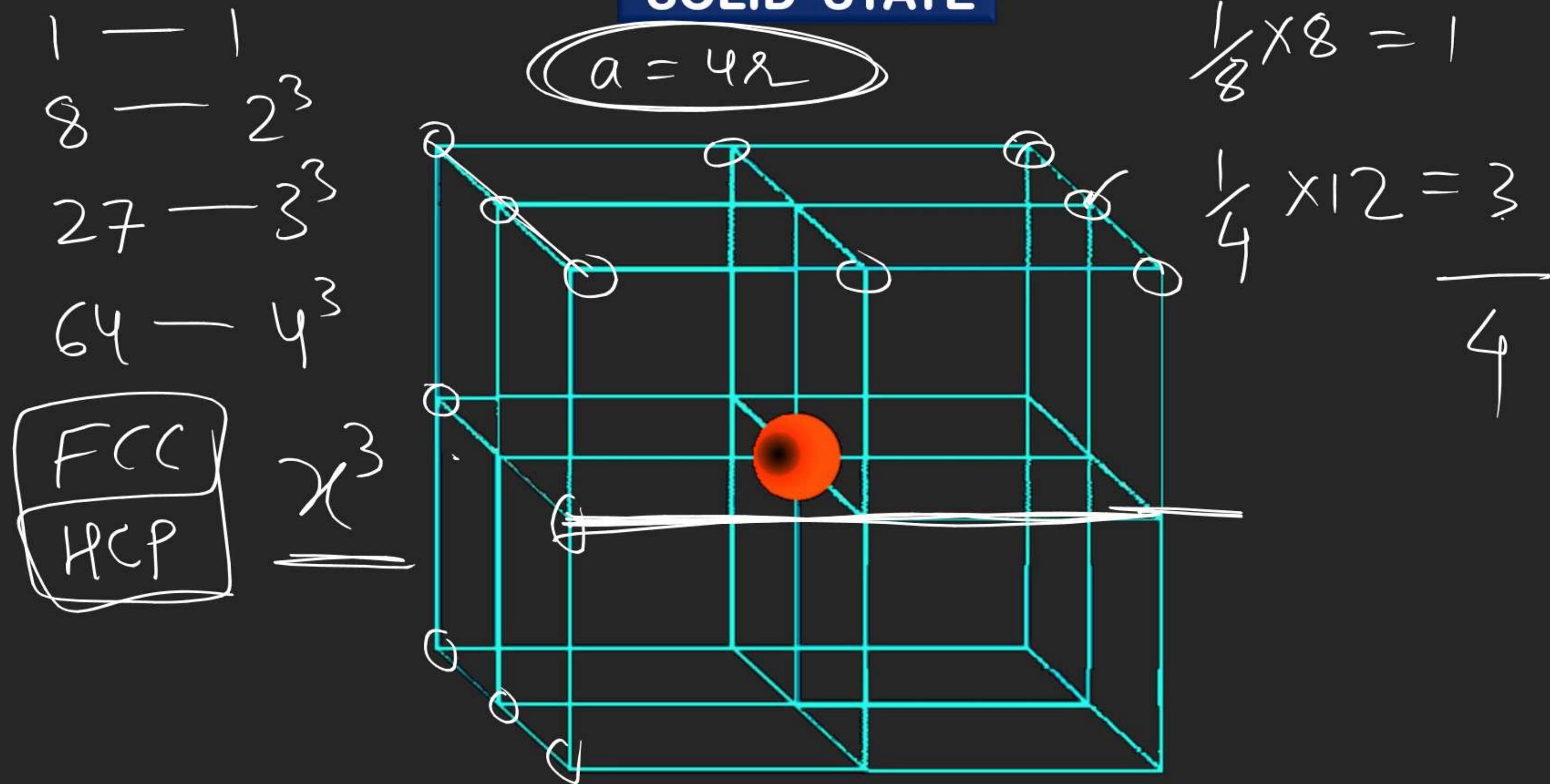
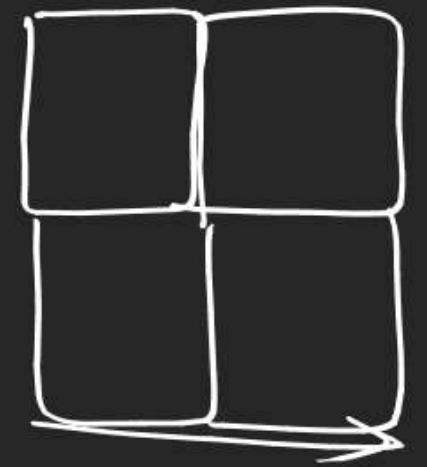


# SOLID STATE

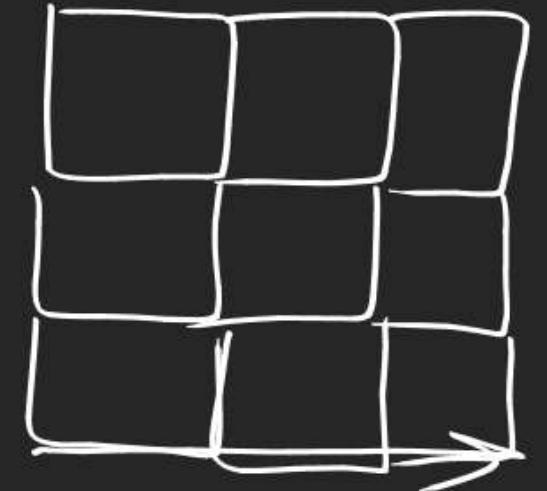




1



$2^2$

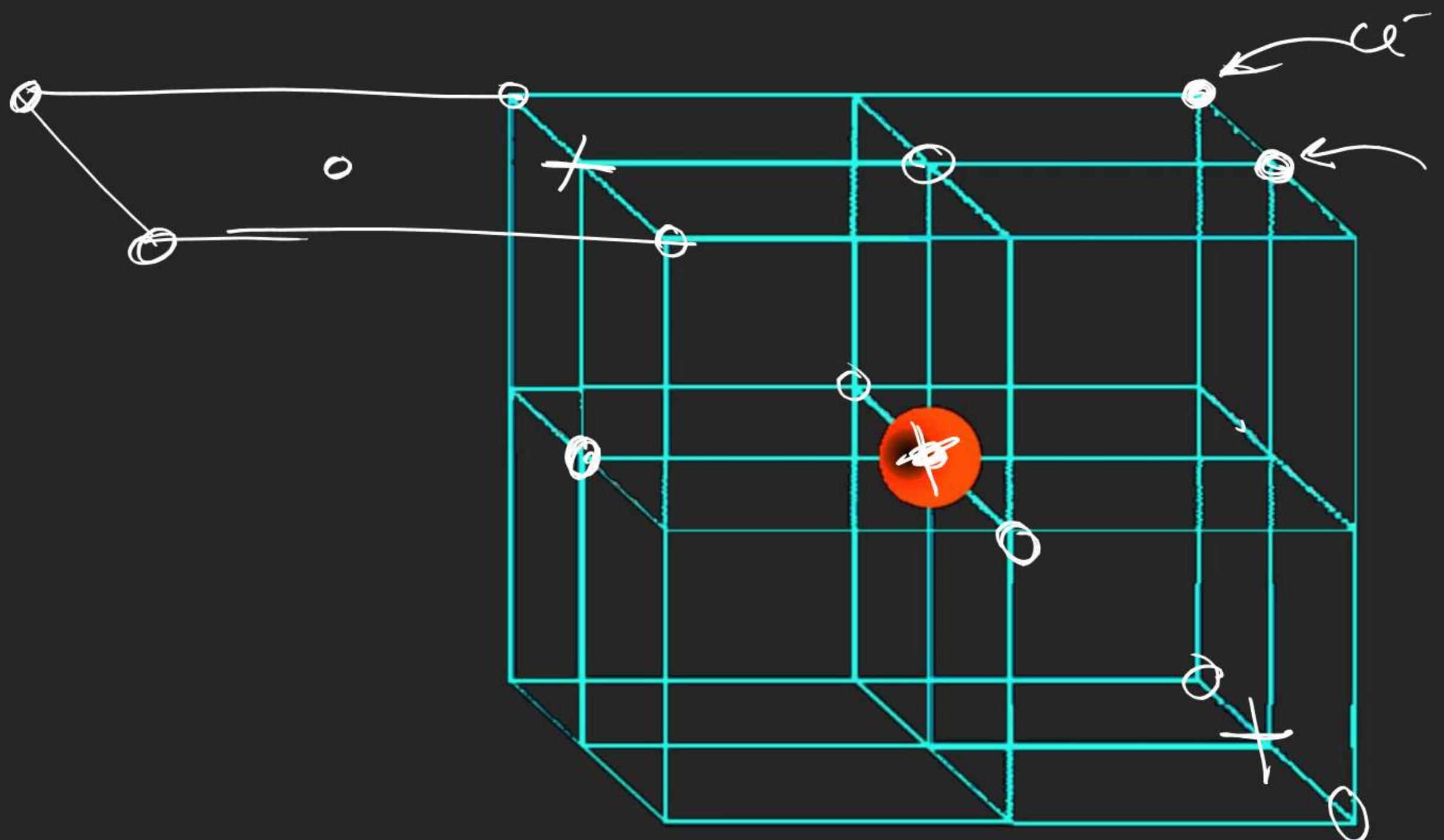


$3^2$

$4^2$

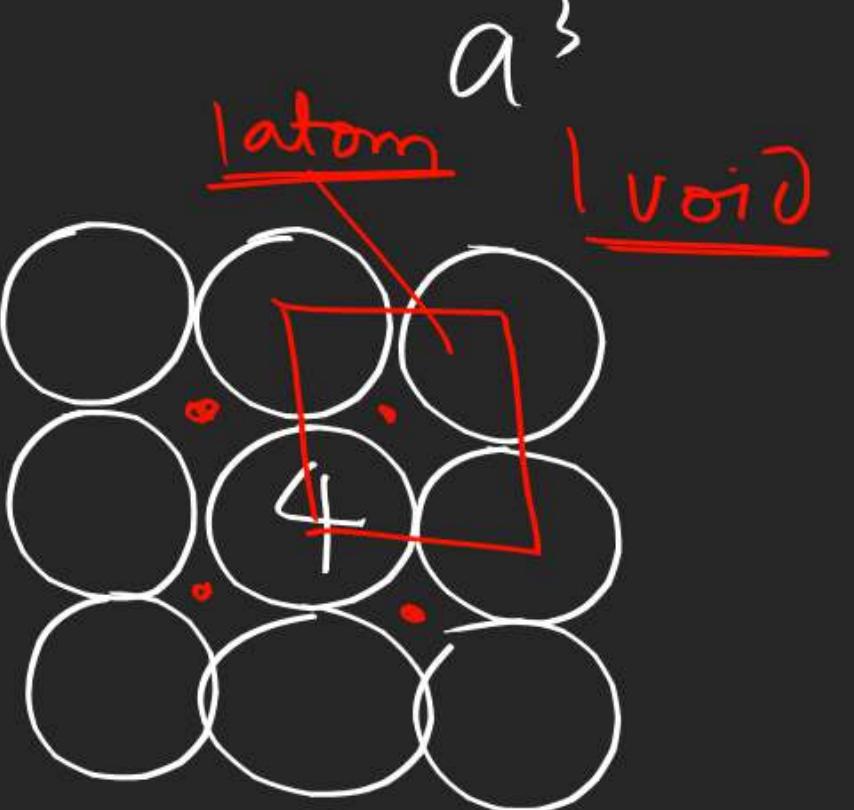
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# SOLID STATE

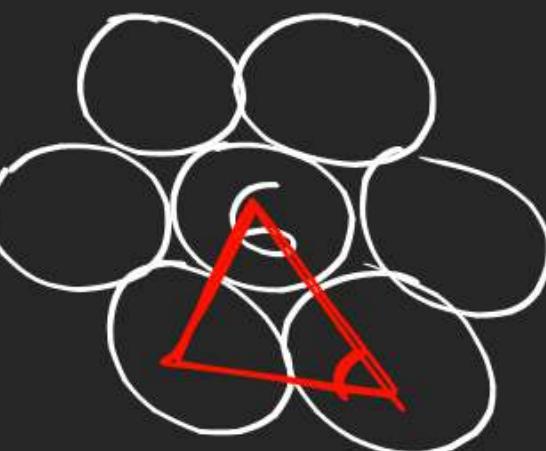


$$d = \frac{Z \times M_{CaF_2}}{N_A}$$

(5)

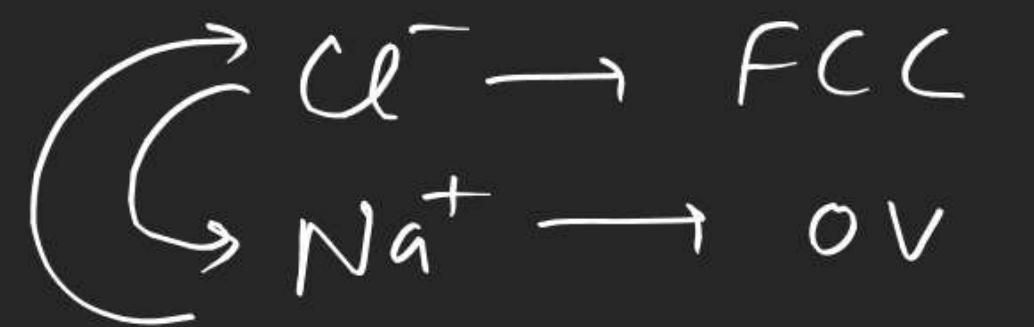


per atom 2 voids



$$= \frac{1}{6} \times 3 \quad \underline{\text{void}}$$

$$= \frac{1}{2} \text{ atom} \quad \underline{\underline{\text{atom}}}$$



②

A

FCC

B

O.V

4

4

$$\begin{cases}
 \text{4 corner} \\
 \text{2 Face centres} \\
 \rightarrow 4 \times \frac{1}{8} + 2 \times \frac{1}{2} \\
 = \frac{1}{2} + 1 \\
 = \underline{\underline{1.5}}
 \end{cases}$$

B - cube centre = 1

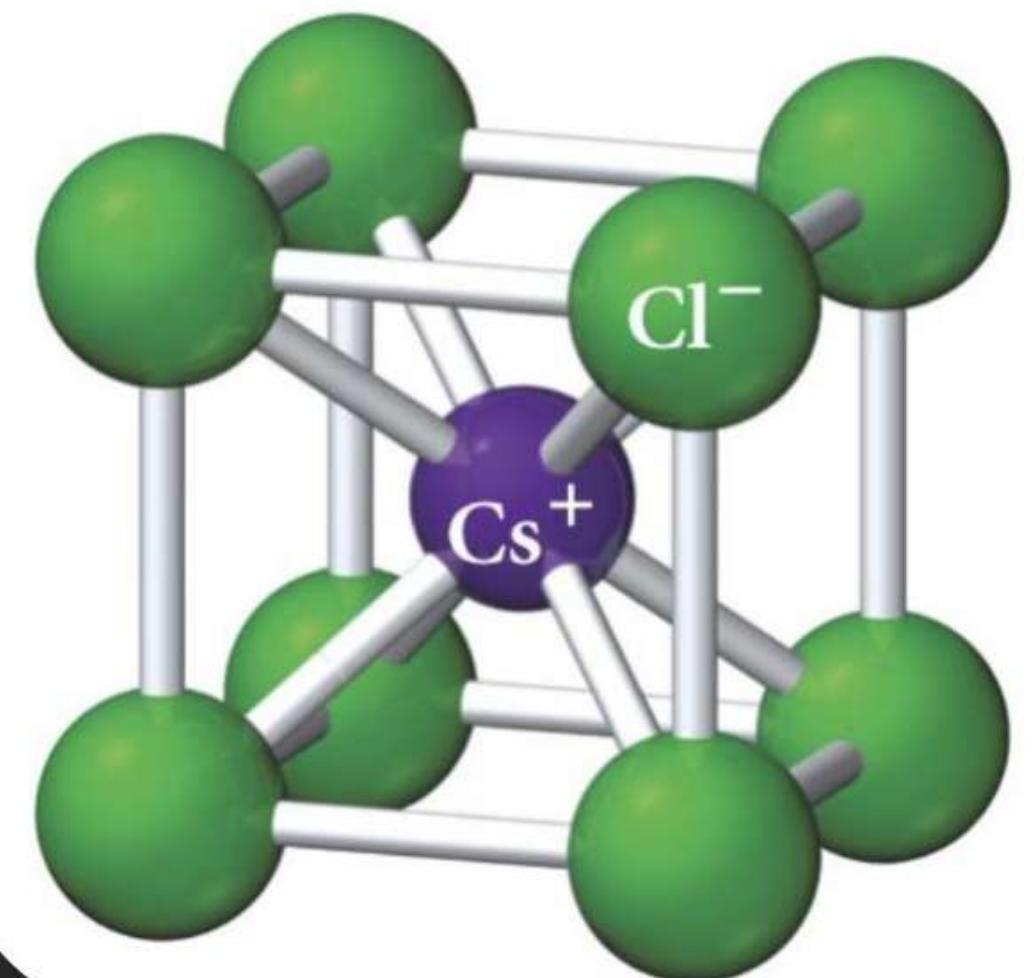
2 edge cent

$$2 \times \frac{1}{4} = \frac{1}{2}$$

$$= \underline{\underline{1.5}}$$

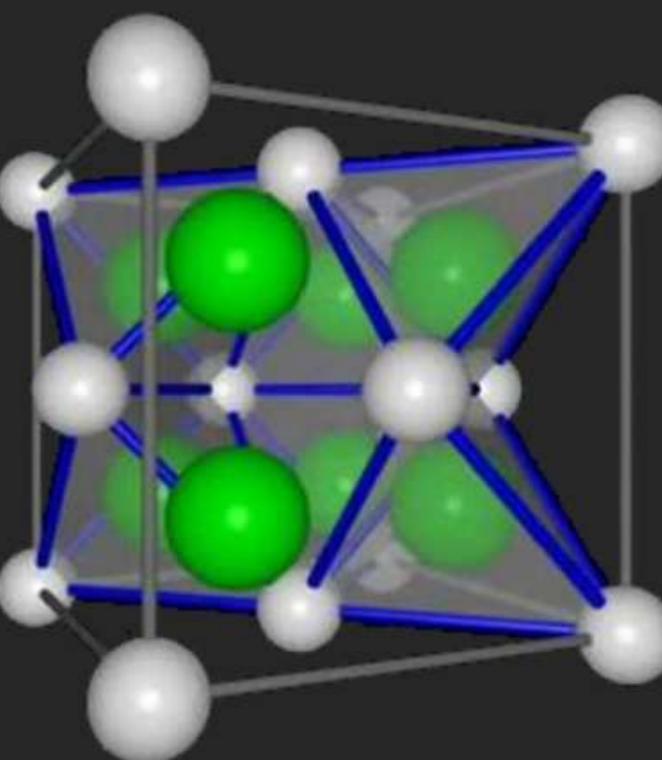
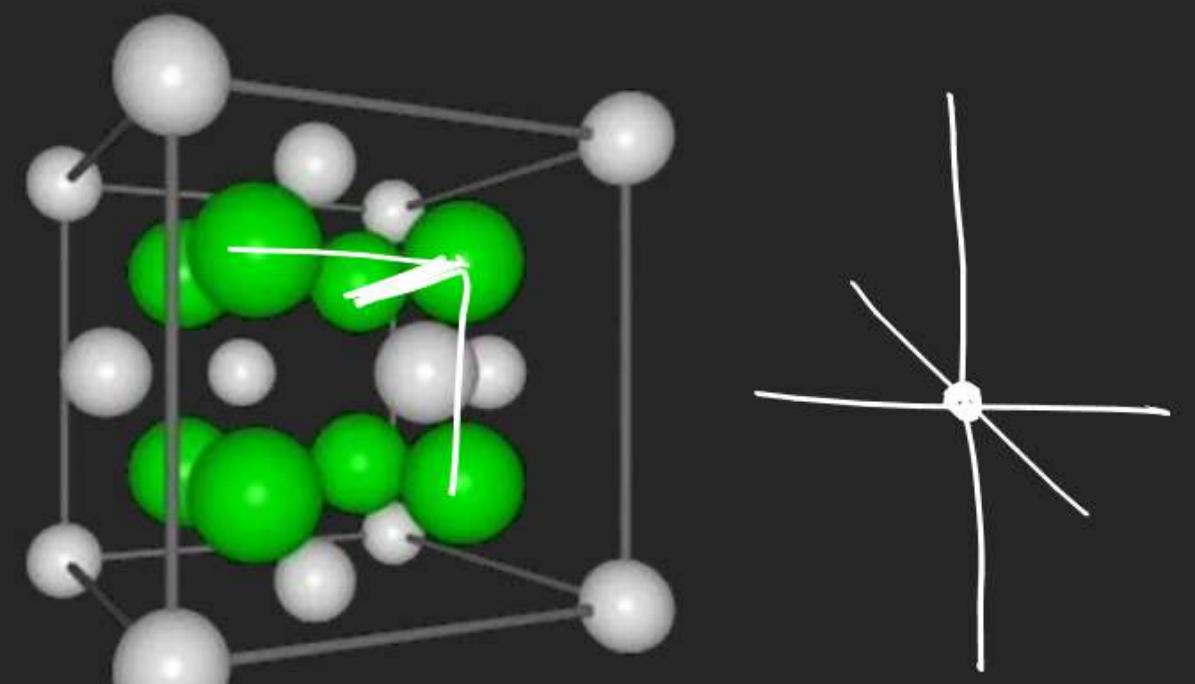
# SOLID STATE

Cesium chloride ( $\text{CsCl}$ )



# SOLID STATE

Fluoride Ions Occupy Tetrahedral Holes



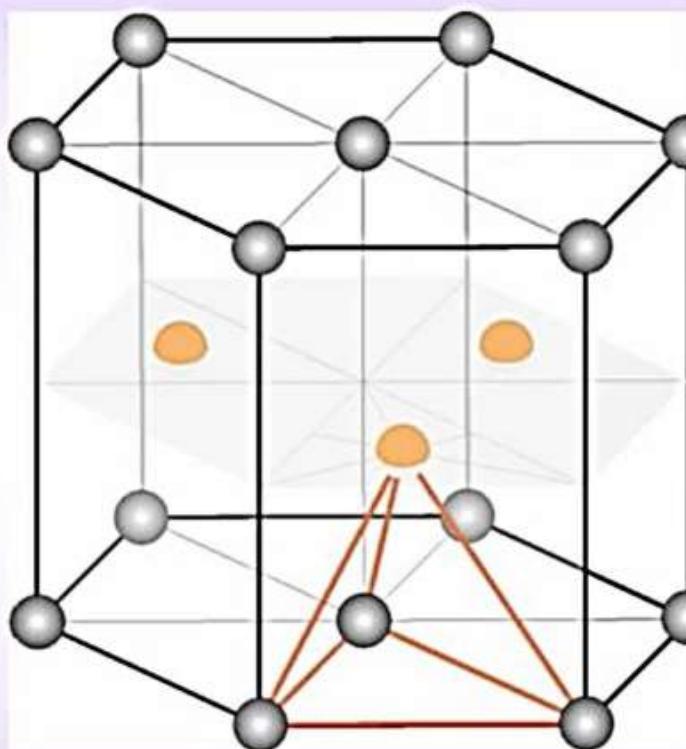
# SOLID STATE

HCP

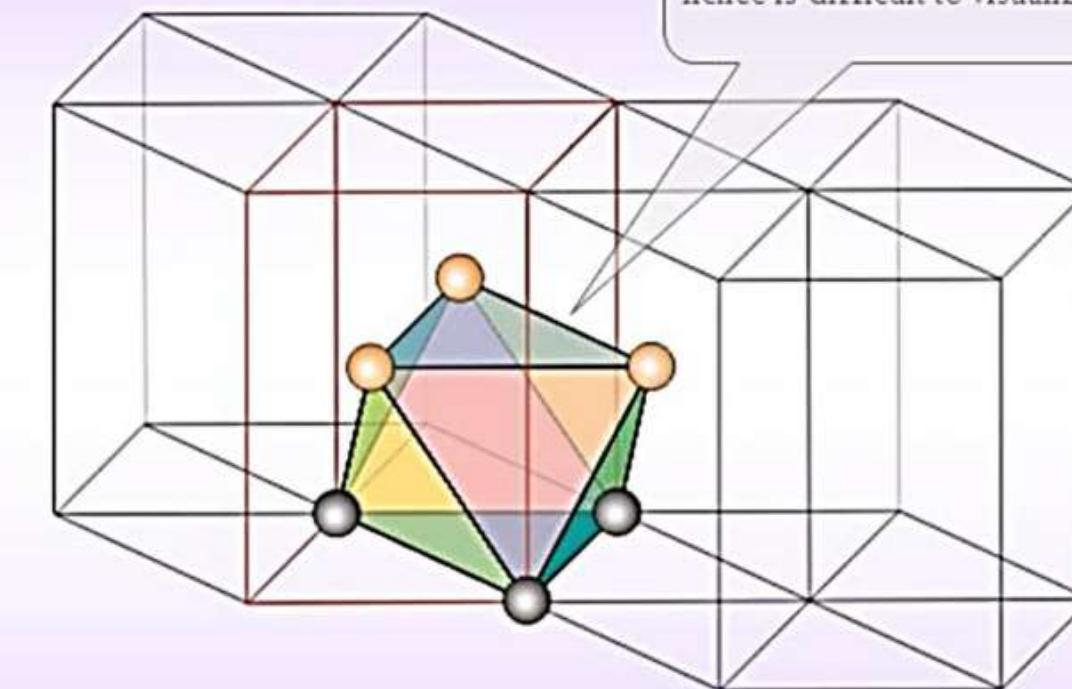
VOIDS

TETRAHEDRAL

OCTAHEDRAL



Coordinates:  $(0, 0, \frac{3}{8}), (0, 0, \frac{5}{8}), (\frac{2}{3}, \frac{1}{3}, \frac{1}{8}), (\frac{2}{3}, \frac{1}{3}, \frac{7}{8})$



Coordinates:  $(\frac{1}{3}, \frac{2}{3}, \frac{1}{4}), (\frac{1}{3}, \frac{2}{3}, \frac{3}{4})$

- These voids are identical to the ones found in FCC (*for ideal c/a ratio*).
- When the c/a ratio is non-ideal then the octahedra and tetrahedra are distorted (*non-regular*).

**Important Note:** often in these discussions an ideal c/a ratio will be assumed (without stating the same explicitly).

*If c/a ratio is not the ideal one – then the voids will not be ‘regular’ (i.e. regular octahedron and regular tetrahedron).*

O-I      ③5      8 : 8

CsCl type       $\frac{\sqrt{3}a}{2} = r_+ + r_-$

③8       $\frac{r_+}{r_-} = 0.225$

NaCl

6 : 6

ZnS

4 : 4

S-I ②8

$$a = 2\lambda_-$$

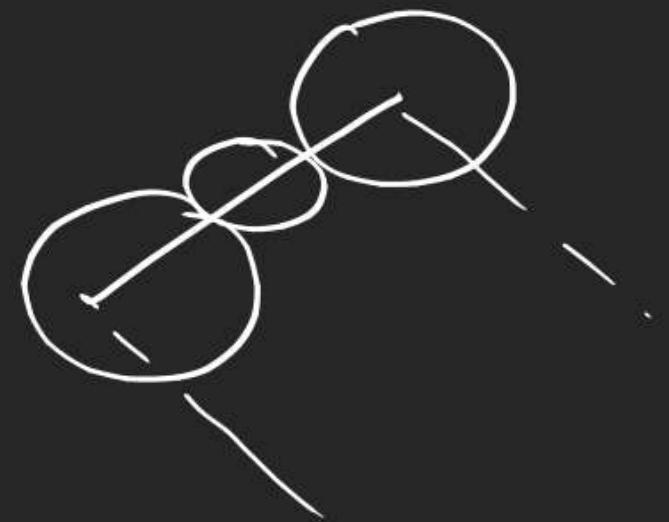
$$a = 2 \times 2.17 \text{ \AA}^0$$

②7

$$\begin{aligned}\sqrt{3}a &= 2\lambda_+ + 2\lambda_- \\ &= 7 \text{ \AA}^0\end{aligned}$$

②6

$$\frac{\sqrt{3}a}{2} = \lambda_+ + \lambda_- = \underline{200\sqrt{3} \text{ Ang}}$$



$$\text{height} = 2r$$

$$\text{length} = 4r$$



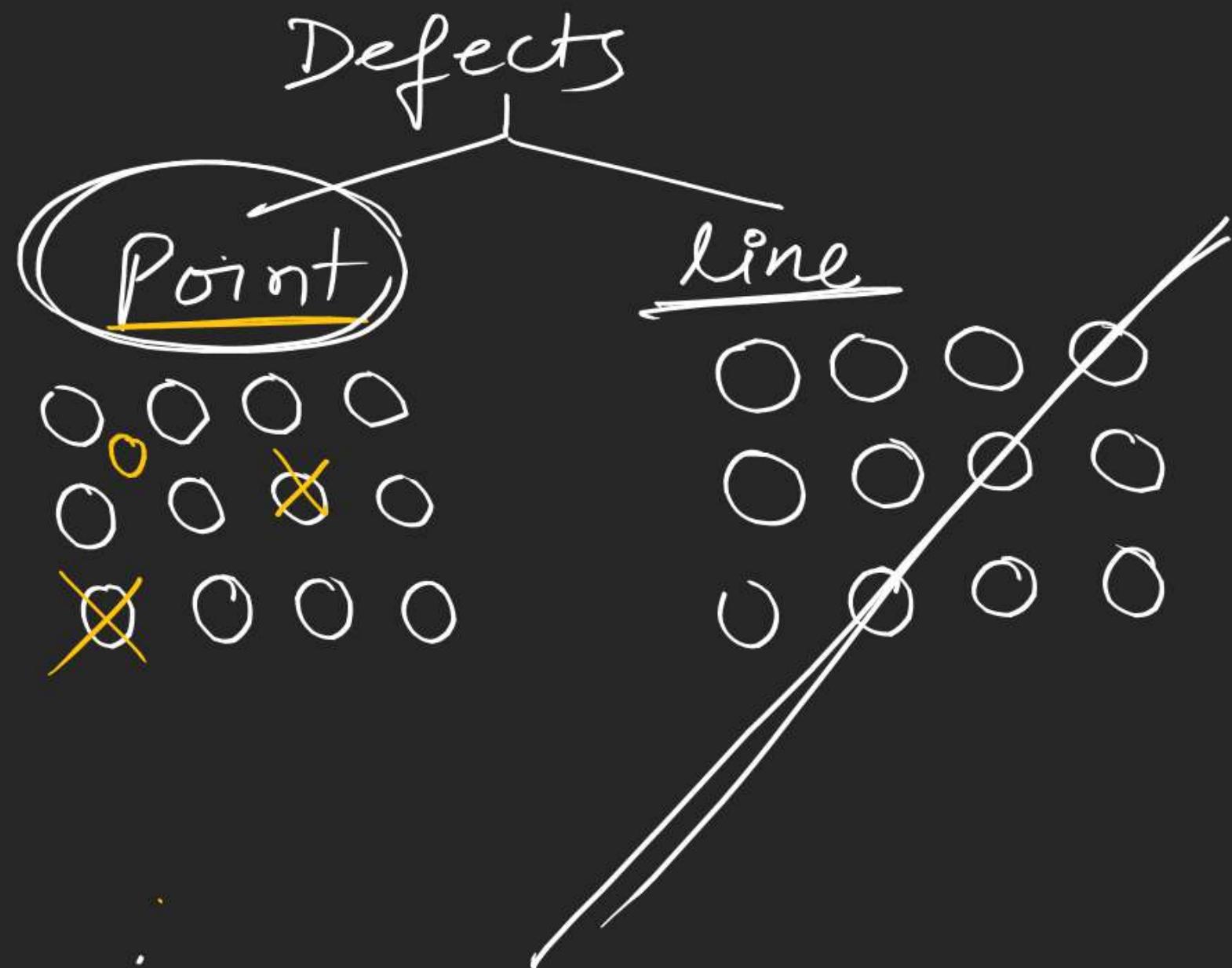
$$\text{Area} = (4r)^2$$

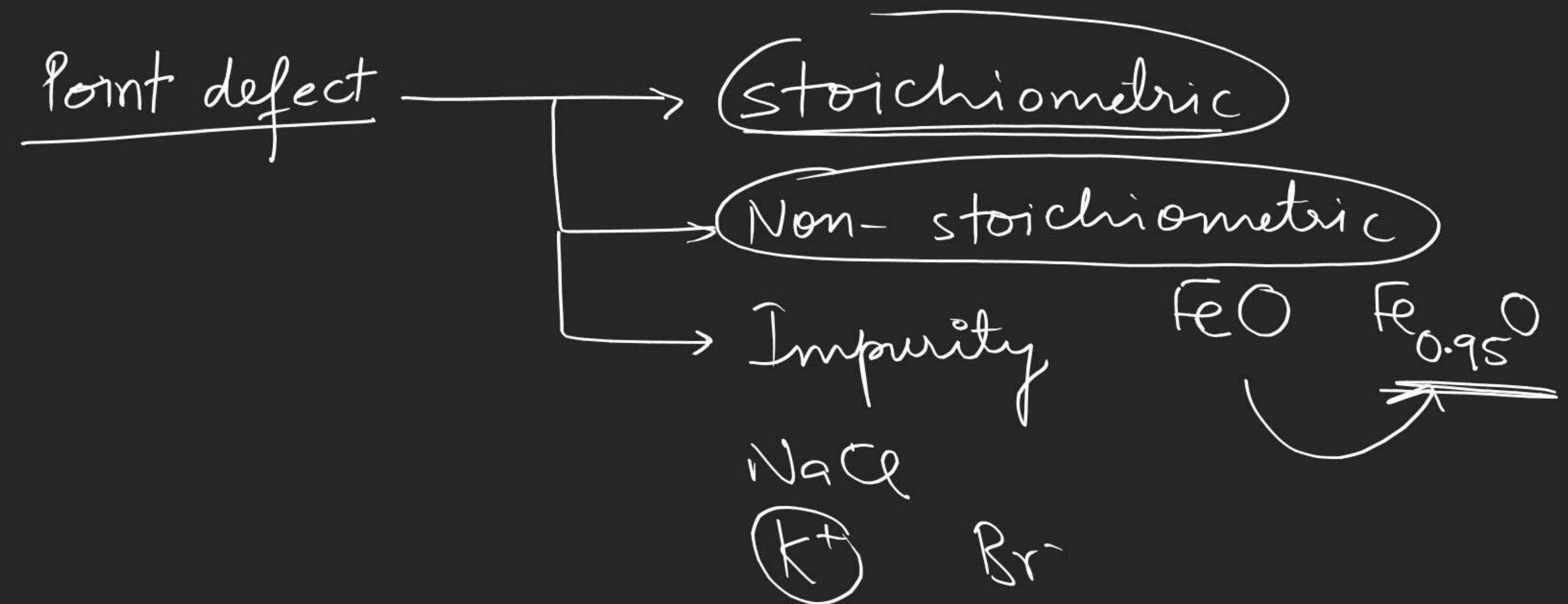
$$\text{Volume} = 32r^3$$

$$\text{PF} = \frac{4 \times 4/3 \pi r^3}{32 r^3} \times 100 = \frac{\pi}{6} \times 100$$

$$= 100 - \frac{\pi}{6} \times 100$$

Defects :→ Deviation from ideal arrangement

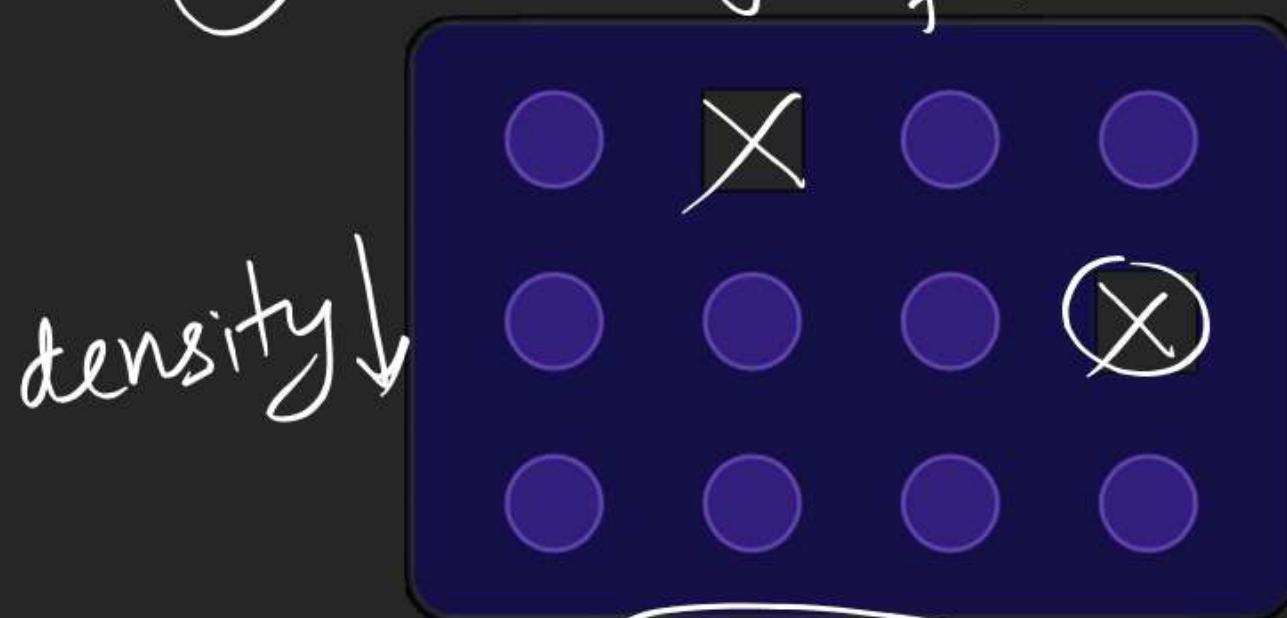




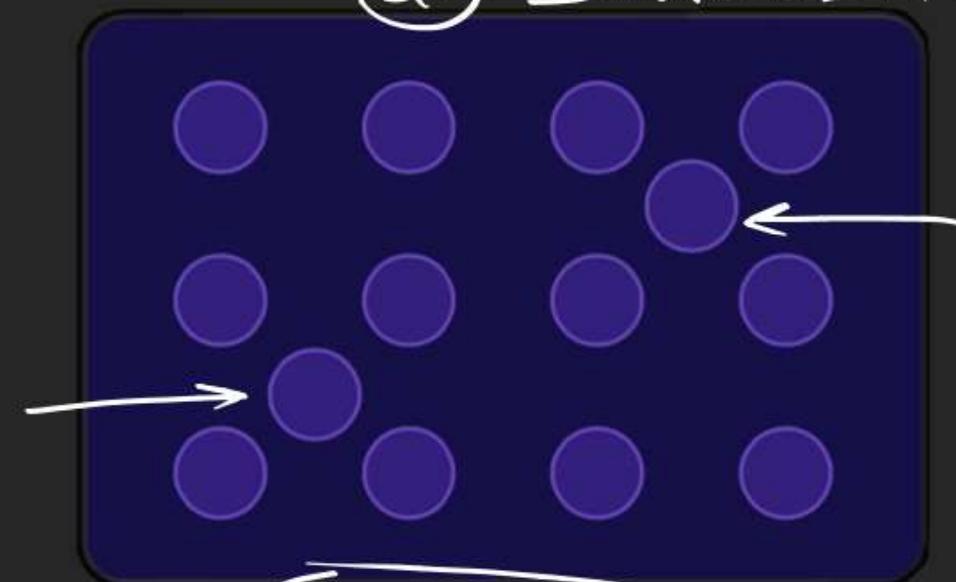
stoichiometric defect :  $\rightarrow$  formula of the compound remains same

# SOLID STATE

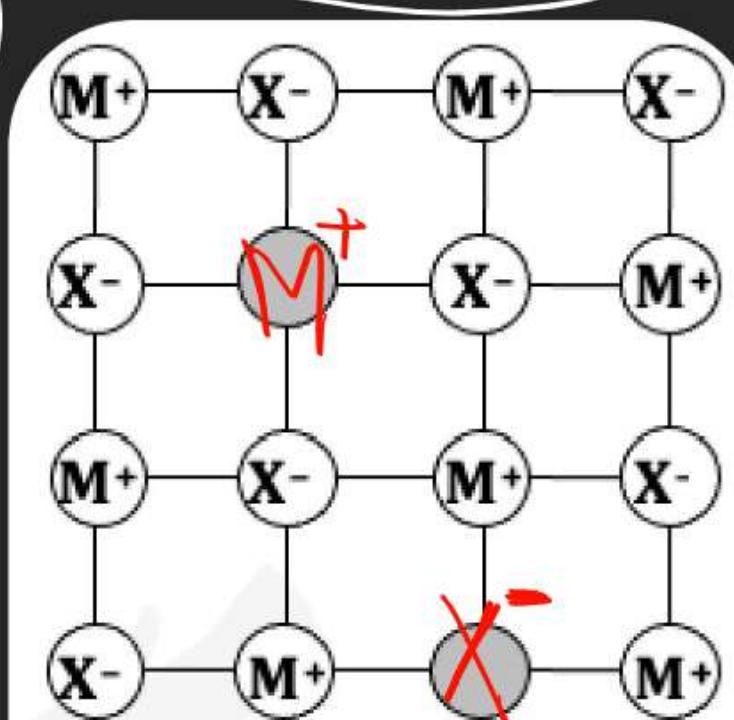
① Vacancy defect



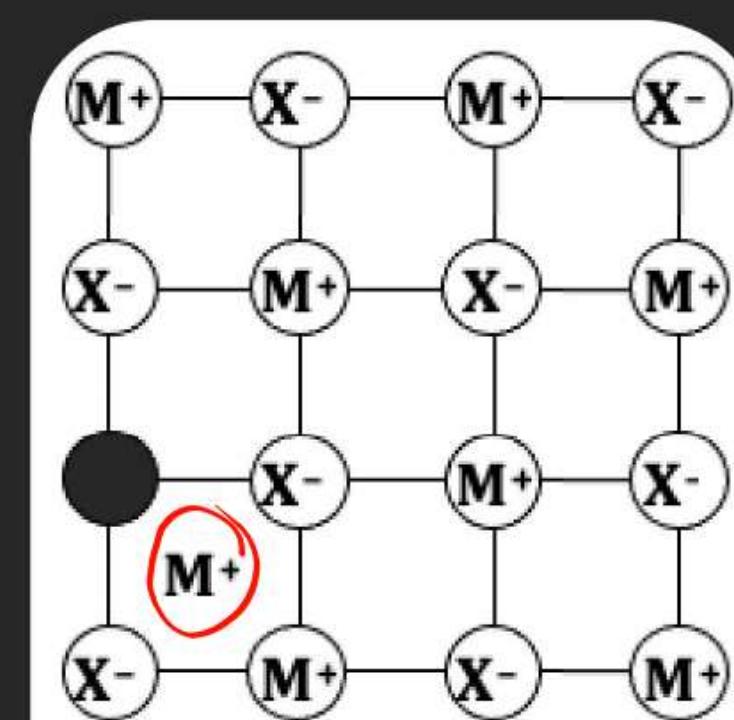
② Interstitial defect



$GaF_2$

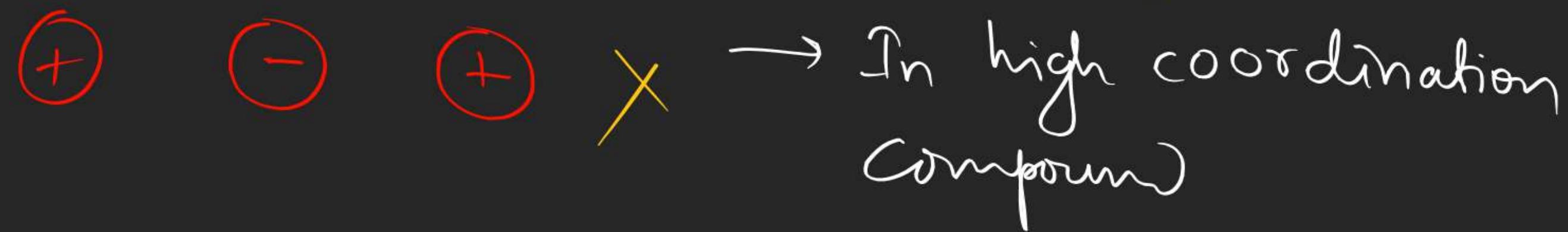
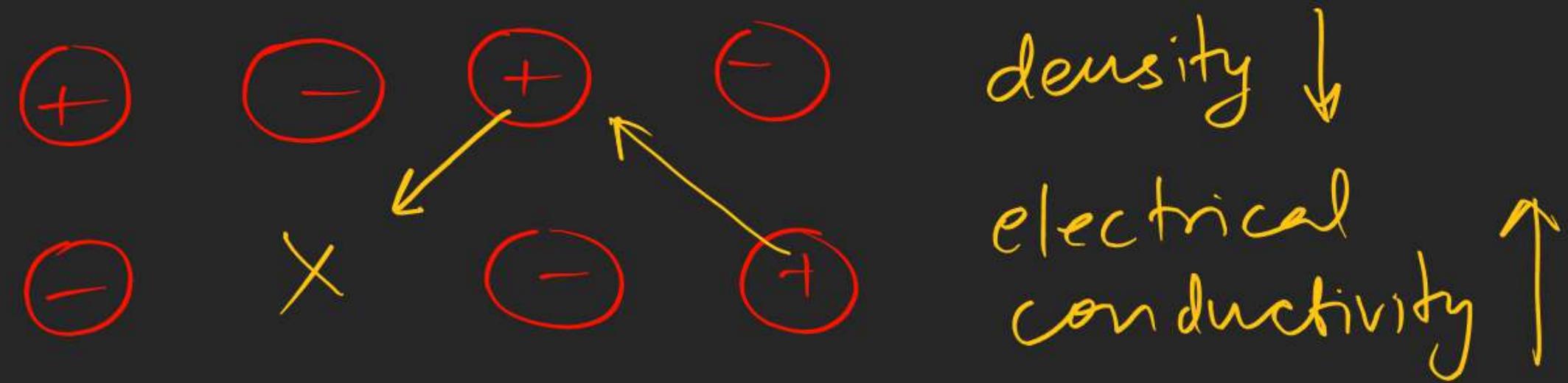


Schottky Defect



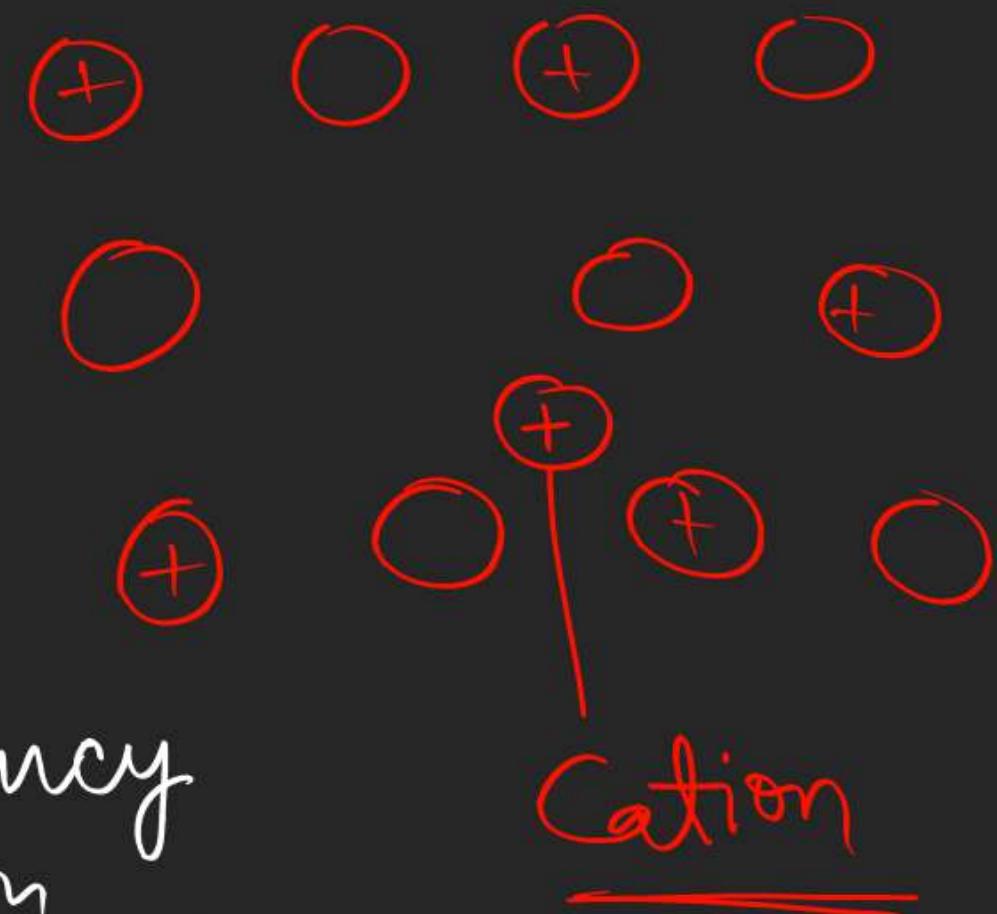
Frenkel Defect

Schottky defect :  $\rightarrow$  exist in ionic compound



e.g.  $\text{CsCl}$

Frenkel defect :  $\rightarrow$  dislocation defect



density — Same

electrical conductivity  $\uparrow$

$\rightarrow$  Mainly observed in  
low co-ordination no.  
compound e.g ZnS



Non-stoichiometric defect :  $\rightarrow$

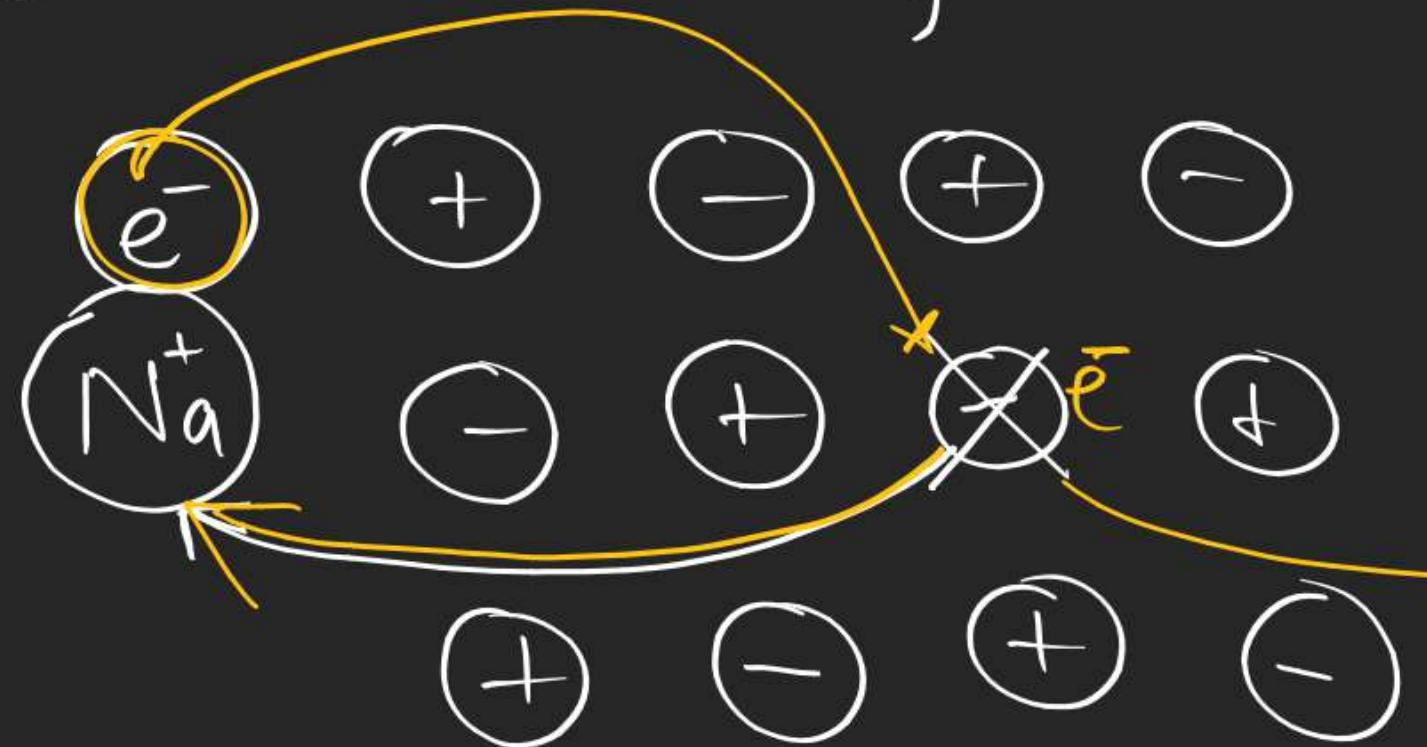
Cation-metal ion

① Metal excess  
defect

② metal  
deficiency  
defect



① Metal excess defect due to anionic vacancies



density ↓

electrical conductivity ↑

F - centre

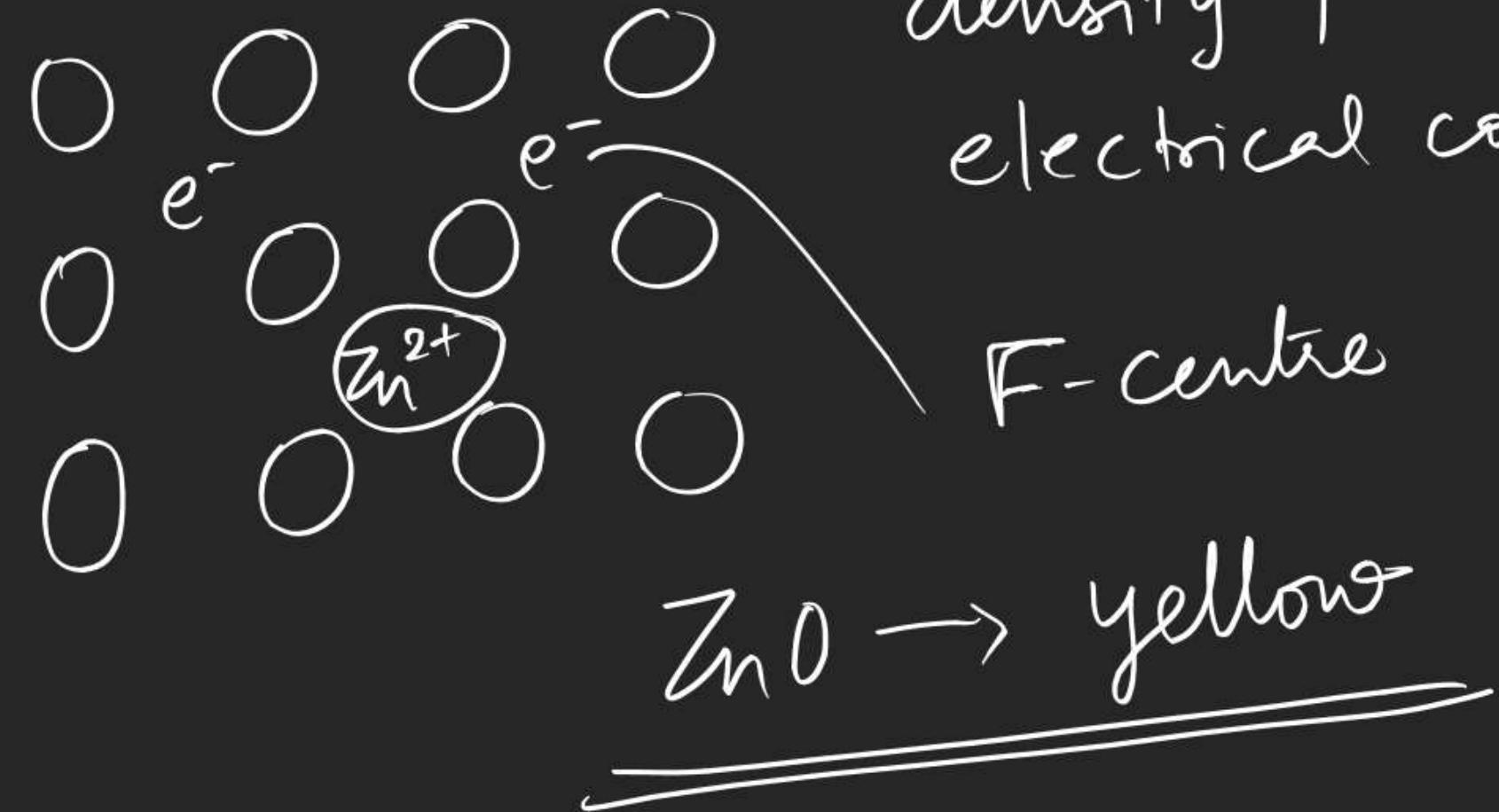
Farbe

(Colour)

- $\text{NaCl}$  — Yellow
- $\text{LiCl}$  — Pink
- $\text{KCl}$  — violet (lilac)

⑪ Metal excess defect due to extra metal ion

e.g.  $\text{ZnO}$

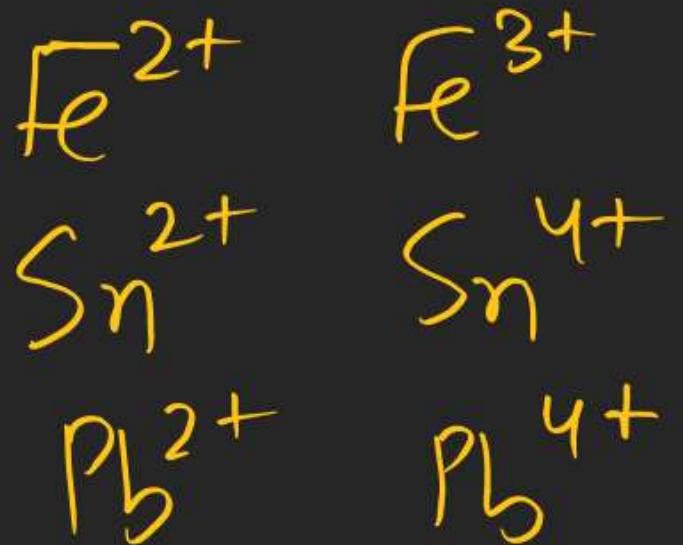
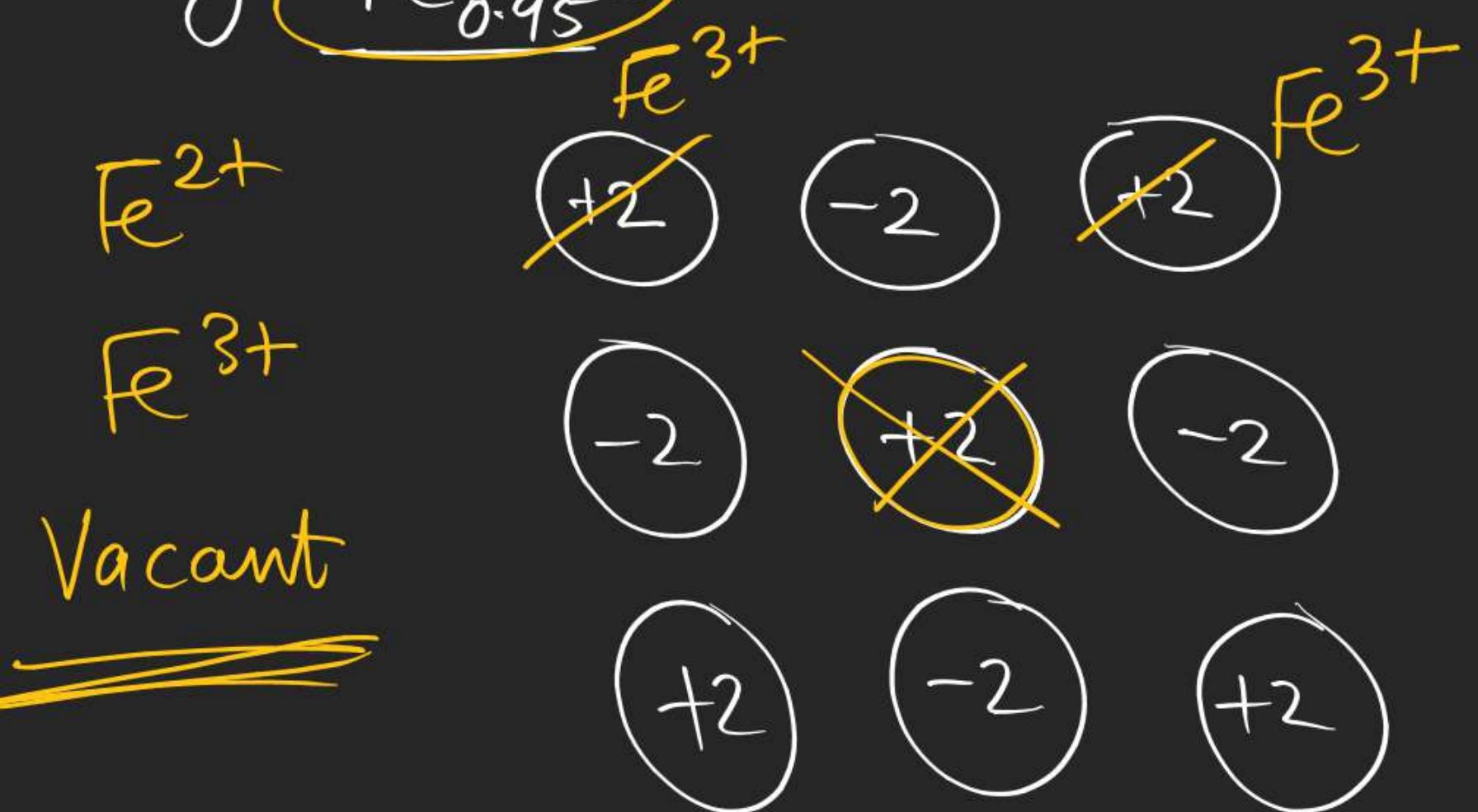


density ↑  
electrical conductivity

$\text{ZnO} \rightarrow \text{yellow}$

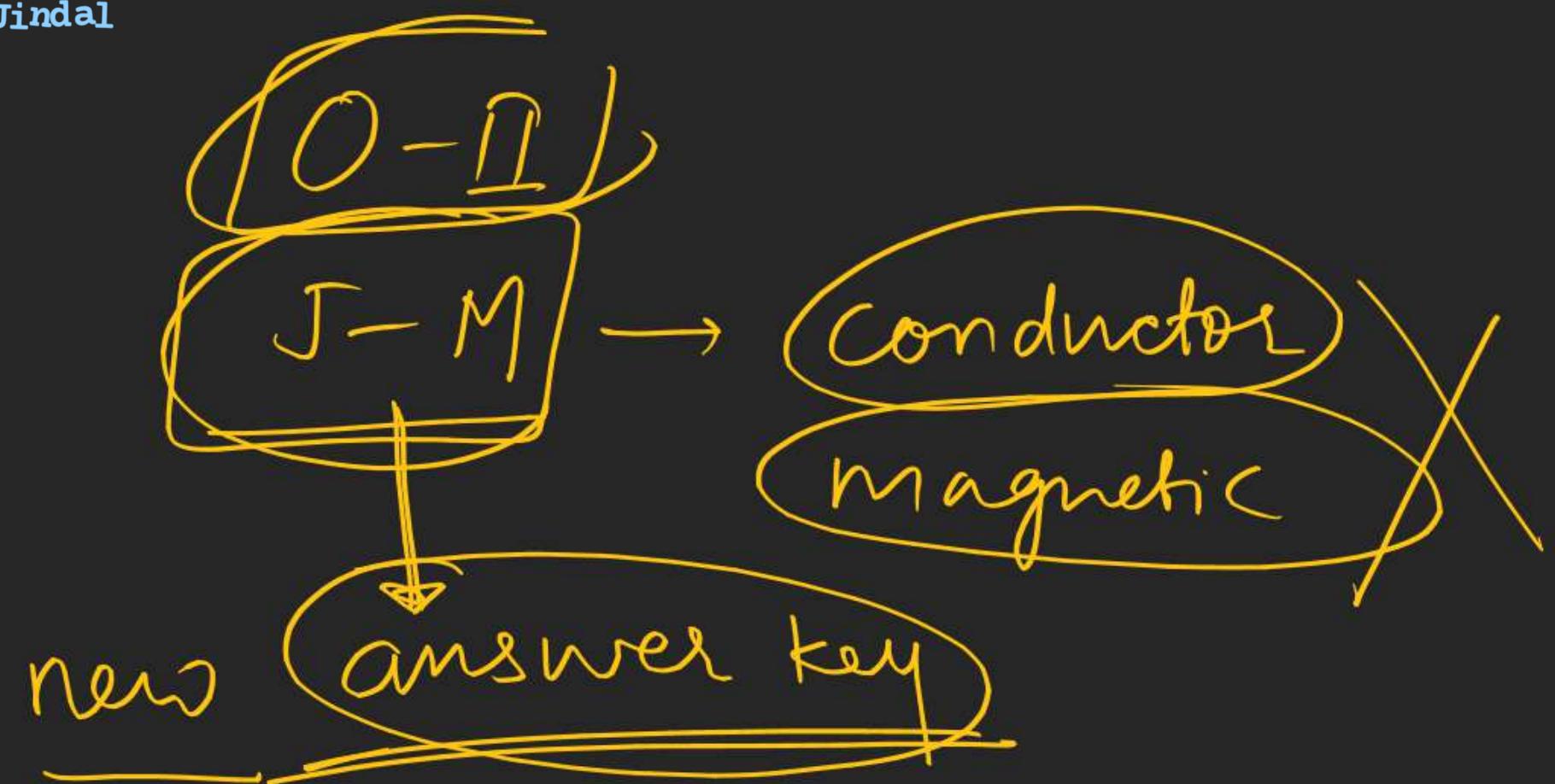
### ③ Metal deficiency defect due to missing cation

e.g.



1 Vacancy  $\Rightarrow +2$

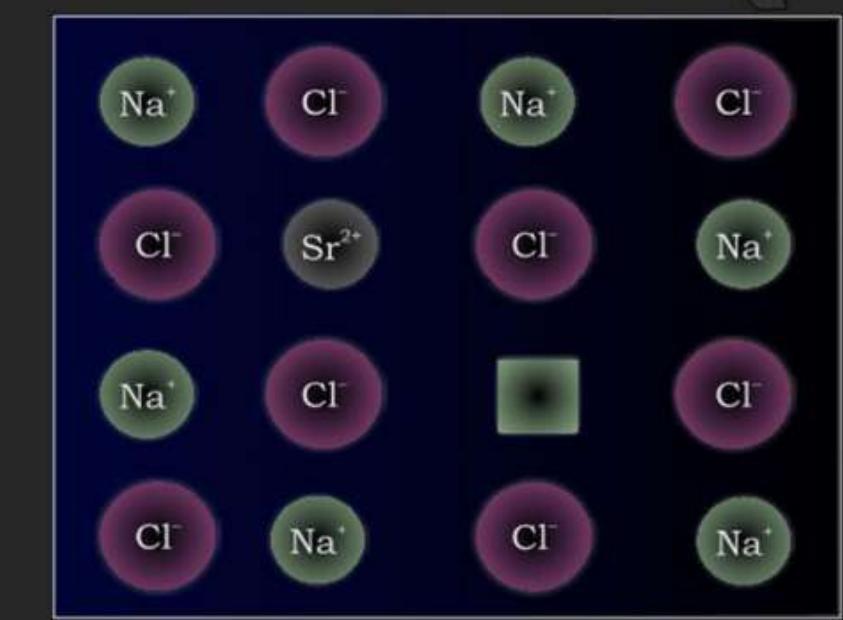




# SOLID STATE



An F-centre in a crystal



**Fig. 1.31:** Introduction of cation vacancy in  $\text{NaCl}$  by substitution of  $\text{Na}^+$  by  $\text{Sr}^{2+}$