

Day-27

→ Ionic defects → defect chemistry

↓
Notation

→ Internal → Bulk of the material
 ↘
 higher dimensional defects

→ cation: anion ratio remains same in stoichiometric defect

↓
No higher dimensional (or 1D)
(• Frenkel → cation sub-lattice
• Anion Frenkel → silver halide)
↓
higher-D defect is involved
↓
schottky defect (NaCl)

→ Building block notation of ionic defects (point): $\text{NiI} \leftrightarrow \text{Ag}^+ + |\text{Ag}|^-$

→ Kröger-Vink Notation:

Any defect - M_s^c → Relative charge
 ↓
 structural element
 ↓
 Interstitial or regular position
 ↓
 ~~(X)~~

★ For AgCl:

V_{Ag}^+ → silver site
charge on that site → +1 (0 - (+1))

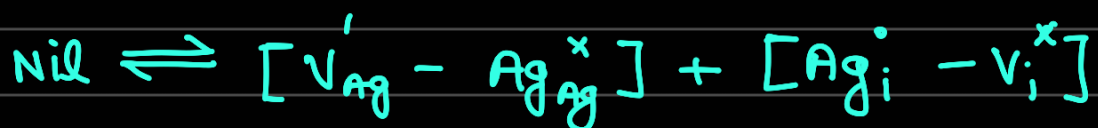
$V'_{Ag} \rightarrow$ A singly ionized vacancy on a silver site.

\downarrow
-vely charged ionic defined.

$V^{\bullet}_{Cl} \rightarrow$ singly ionized chlorine vacancy



$\bullet \rightarrow$ no charge associated



\rightarrow mass Action Law:

$[V'_{Ag}] \rightarrow$ concentration of singly ionized silver vacancies
Electroneutrality condition (ENC)

$$\downarrow$$

$$[V'_{Ag}] = [Ag_i]$$

$$K_F = \frac{[V'_{Ag}][Ag_i]}{[Ag^{\bullet}_{Ag}][V^{\bullet}_i]} = Q = e^{\frac{-\Delta G_F^{\circ}}{RT}} = e^{\frac{-\Delta H_F^{\circ}}{RT} + \frac{\Delta S_F^{\circ}}{R}}$$

\downarrow \downarrow \uparrow 140 kJ/mol \uparrow 9.4R
 N $\propto N$ Q Q

Plot is at particular activity of Ag and partial pressure of Cl.