Day-26

→ Point defects

Equilibrium concentration of vacancies in a metallic crystal

$\exp\left(-\frac{\Delta F_f}{RT}\right)$ → different for different materials

→ Local Electroneutrality condition (ENC)

+ve defect compensated by −ve defect

Kroger-Vink Notation

→ Stoichiometric defect −

Anion-cation ratio is maintained

MX

Cation Anion

FeO (1:1)

consider a region of the perfect crystal

100 FeO
10 vacancies of O
10 vacancies of Fe

90 Fe + 90 O (1:1)

→ Another way: 10 vacancies of oxygen
those 10 oxygen atoms can

go to interstitial positions

(Also a stoichiometric defect)

→ Non-stochiometric defect

$MX \longrightarrow M_{1-y}X \quad (0<y<1)$

100 M and 100 X

Create 10 vacancies of M ($y = 0.1$)

$M_{0.9}X$

Eg: $Fe^{2+}O^{2-}$ $\quad 6Fe^{2+} \longrightarrow 6Fe^{3+}$

→ Interaction between ionic defects and electronic defects

→ Interaction with environment (other than temp. equilibrium)

O → interstitial site

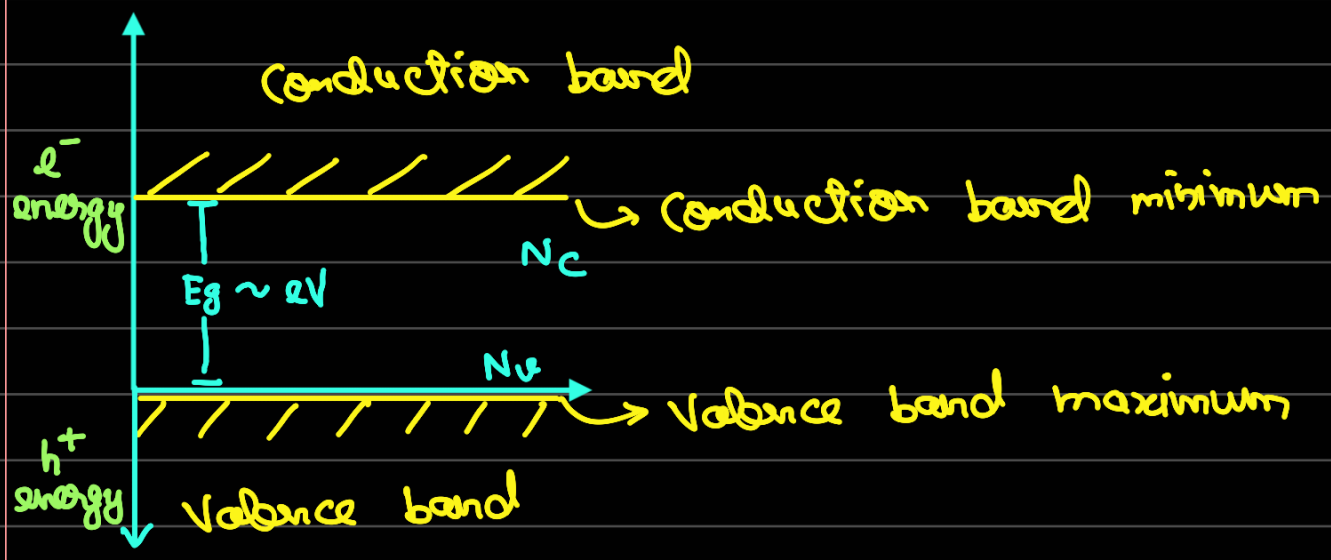
↓

FeO_{1+z}

→ Electron as a defect

Band gap → There are certain values of energy it cannot assume.

Flat Band diagram



Effective density of States

At $T = 0$ K, some n e^-

$n \longrightarrow$ VBM $\rightarrow E = 0$

OR m $e^- \longrightarrow$ CBM $\rightarrow E = (n-m)\,0 + mE_g$

$(n-m)$ $e^- \longrightarrow$ VBM $= mE_g > 0$

If $T > 0$

Energy available $\longrightarrow$ Thermal energy $= KT$

when $T \approx 300$ K, $KT \approx 25$ meV

n e^- at VBM $\longrightarrow$ I

$(n-m)$ e^- at VBM + m at CBM $\longrightarrow$ II

at $T > 0$

n $e^- \longrightarrow$ $2n$ states

$T = 0$ K (perfect state)

$\Delta F = \Delta U - T\Delta S$

T > 0 (defect)

Any e^- in C.B. is considered a defect

(electron) hole $\longrightarrow h$

$$Nil \rightleftharpoons [+] + [-]$$

$$e(VB) + h(CB) \rightleftharpoons [e(CB)] + [h(VB)]$$