3.46 PHOTONIC MATERIALS AND DEVICES

Lecture 14: Defects and Strain

Lecture Notes

Perfection

- LRO (Long Range Order)
- SRO (Short Range Order)

Imperfection

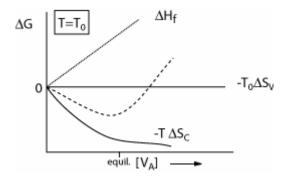
- Vibrating atom
- Electronic change
- Chemical impurity
- Point defect (I, V)
- 1D defect (dislocation)
- 2D defect (grain boundary)
- 3D defect (precipitate)

Defect Chemistry

$$\Delta G_{_{f}} = \Delta H_{_{f}} - T(\Delta S_{_{V}} + \Delta S_{_{C}})$$

Vacancy Equilibria

$$\mathsf{A}_\mathsf{A} \rightleftarrows \mathsf{V}_\mathsf{A} + \mathsf{A}_\mathsf{A}$$



Notes

Charge Carriers as Defects

$$\begin{split} e^- + h^+ &\rightleftarrows bond \\ \left[e^- \right] \! \left[h^+ \right] \! = np = K_{np} \\ &= exp \, \left(-\frac{\Delta G}{k_B T} \right) \\ &= exp \left(\frac{\Delta S}{k_B} \right) \, exp \, \left(-\frac{\Delta H}{k_B T} \right) \\ &= N_C N_V \, exp \, \left(-\frac{E_g}{k_B T} \right) \end{split}$$

Point Defect Equilibria in Compounds

$$bB + cC \rightleftharpoons dD + eE$$

$$K = \frac{[D]^{d}[E]^{e}}{[B]^{b}[C]^{c}}$$

AB_x Compounds

Schottky Defect (vacancy pair)

$$\begin{split} \boldsymbol{A}_{A} + \boldsymbol{x} \boldsymbol{B}_{B} & \rightleftharpoons \boldsymbol{V}_{A} + \boldsymbol{x} \boldsymbol{V}_{B} + \boldsymbol{A}_{A} + \boldsymbol{B}_{B} \\ \boldsymbol{K}_{S} & = \big[\boldsymbol{V}_{A}\big] \big[\boldsymbol{V}_{B}\big]^{x} \end{split}$$

Frenkel Pair

$$\begin{split} \boldsymbol{A}_{A} &\rightarrow \boldsymbol{A}_{I} + \boldsymbol{V}_{A} \\ \boldsymbol{K}_{FP} \left(\boldsymbol{A} \right) = \left[\boldsymbol{A}_{I} \right] \! \left[\boldsymbol{V}_{A} \right] \\ \boldsymbol{K}_{FP} \left(\boldsymbol{B} \right) = \! \left[\boldsymbol{B}_{I} \right] \! \left[\boldsymbol{V}_{B} \right] \end{split}$$

Anti-Site Defect

$$\begin{aligned} \mathsf{A}_{\mathsf{A}} + \mathsf{B}_{\mathsf{B}} & \rightleftharpoons \mathsf{A}_{\mathsf{B}} + \mathsf{B}_{\mathsf{A}} \\ \mathsf{K}_{\mathsf{AS}} &= [\mathsf{A}_{\mathsf{B}}][\mathsf{B}_{\mathsf{A}}] \end{aligned}$$

Notes

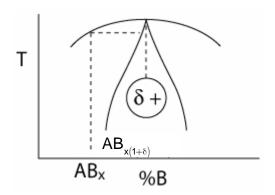
Nonstoichiometry

$$\begin{split} &AB_{x} \\ &\frac{\left[A\right]}{\left[B\right]} \neq \frac{1}{x} \\ &\Rightarrow AB_{x(1+\delta)} \end{split}$$

for a volatile component "B"

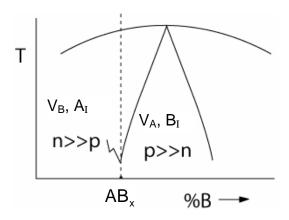
$$\boldsymbol{x}\boldsymbol{\delta} = \! \left[\boldsymbol{A}_{_{\mathrm{I}}}\right] \! - \! \left[\boldsymbol{V}_{_{\!\boldsymbol{B}}}\right] \! + \! \left[\boldsymbol{A}_{_{\!\boldsymbol{B}}}\right]$$

T $AB_{x(1+\delta)}$ AB_x



Electrical Properties: Defect Ion Approximation

A (metal)	B (non-metal)
excess A (δ < 0)	excess B (δ > 0)
V _B (donor)	V _A (acceptor)
A _I (donor)	B _I (acceptor)
A _B (acceptor)	B _A (donor)



Defect-Carrier Equilibria

$$D \mathop{\rightleftharpoons}\limits D^{z+} + ze^-$$

$$A \rightleftharpoons A^{Z-} + zh^+$$

$$\Rightarrow solubility \, \equiv \, f \, (E_F)$$

example: Li in Si (B)

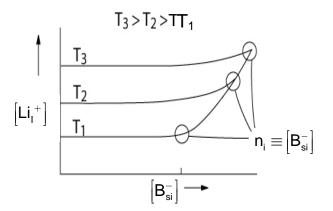
$$\mathsf{B}_{\mathsf{Si}} {\;\rightleftarrows\;} \mathsf{B}_{\mathsf{Si}}^{\scriptscriptstyle{-}} + \mathsf{h}^{\scriptscriptstyle{+}}$$

$$\text{Li}(\text{ext})
ightleftharpoons \text{Li}_{\scriptscriptstyle I}^{\scriptscriptstyle +} + \text{e}^{\scriptscriptstyle -}$$

$$e^- + h^+ \rightleftharpoons bond$$

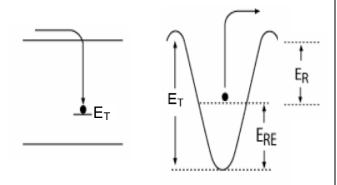
$$\left[B_{s_{i}}^{\scriptscriptstyle{-}}\right]\!+n=\!\left[Li_{_{I}}^{\scriptscriptstyle{+}}\right]\!+p$$

Notes

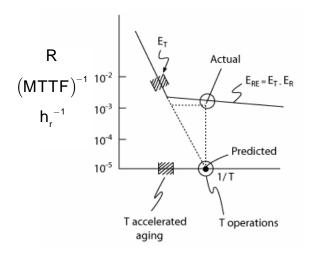


Consequences:

Laser reliability



$$\frac{\mathsf{R}_{\mathsf{RE}}}{\mathsf{R}_{\mathsf{T}}} = \frac{\eta \mathsf{R}_{\mathsf{R}}}{\nu_{\mathsf{L}}} exp \bigg[\frac{\mathsf{E}_{\mathsf{R}}}{\mathsf{k}_{\mathsf{B}} \mathsf{T}} \bigg]$$



Notes

E_R: Recombination Energy

E_T: Transition Energy

E_{RE}: Reaction Enhanced Energy