Prof. M. P. Gururajan
Lec. No. 1
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Phase Field Modelling:

Materials Science, Mathematics and computation

M. P. Gururajan

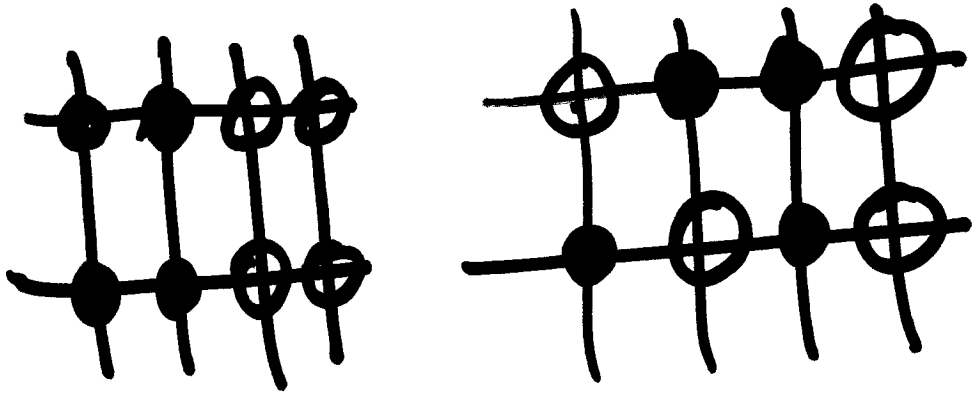
$$G = H - TS$$

Solids / Liquids (PV)

$$H \simeq U$$ Neglect.

$$G \simeq U - TS$$

A B



$$\Delta G^{mix} \simeq \Delta V - T\Delta S$$

Ideal solution

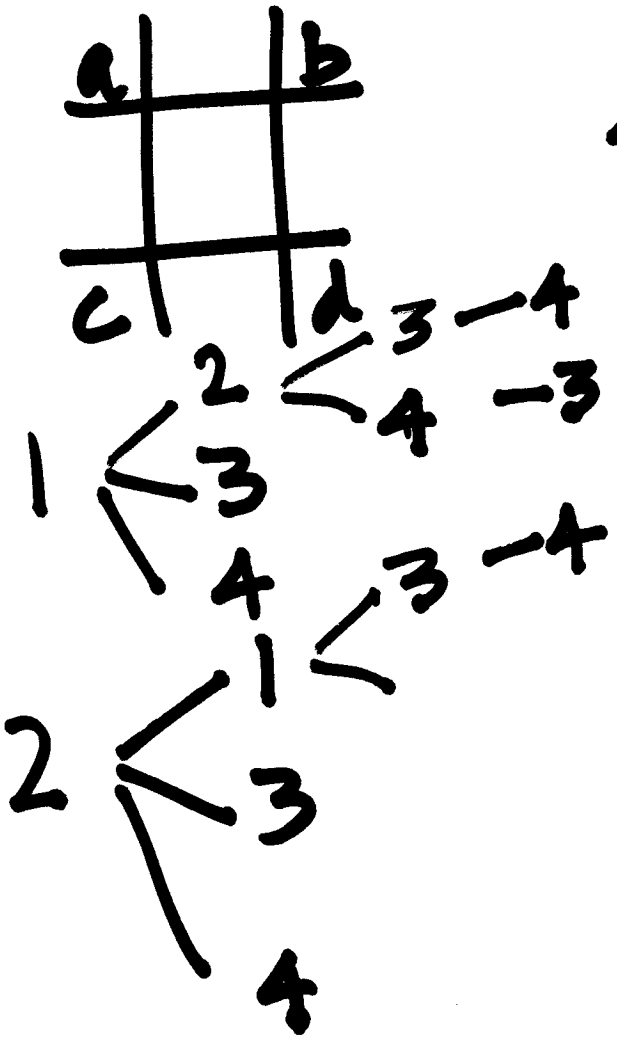
$$\Delta G^{mix} = \underbrace{\Delta U^{mix}}_{\equiv 0} - T\Delta S^{mix}$$

$$\Delta S^{mix} = \Delta S^{mix,\ configurational}$$

$$S = k \ln \omega \qquad N_A,\ N_B$$

$$\omega = \frac{N!}{N_A!\ N_B!} \qquad N = N_A + N_B$$

1, 2, 3, 4 ≡ A



$4 \cdot 3 \cdot 2 \cdot 1 = 4!$

$= 16$

$m+n$

3

$\frac{4!}{4!}$

$\frac{16!}{m!n!}$

4

N = Total # of sites

N_A - atoms of A

N_B - atoms of B

$$N = N_A + N_B$$

$$\omega = \frac{N!}{N_A!\, N_B!}$$

$$\Delta S^{mix,\,config} = k \ln \omega$$

$$-k \ln 1$$

$$-k \ln 1$$

$$\Delta S^{mix,\,config} = k \ln\left(\frac{N!}{N_A!\,N_B!}\right)$$

$$\ln N! = N \ln N - N$$

$$= k\left[\ln N! - \ln N_A! - \ln N_B!\right]$$

$$= k\left[N \ln N - \cancel{N} - N_A \ln N_A + \cancel{N_A} - N_B \ln N_B + \cancel{N_B}\right]$$

$$= -k\left[(N_A + N_B)\ln N - N_A \ln N_A - N_B \ln N_B\right]$$

$$\Delta S^{mix,config} = -k\left[-N_A \ln N - N_B \ln N + N_A \ln N_A + N_B \ln N_B\right]$$

$$= -k\left[N_A \ln \frac{N_A}{N} + N_B \ln \frac{N_B}{N}\right]$$

$$X_A = \frac{N_A}{N}\,; \quad X_B = \frac{N_B}{N} = \underbrace{1 - X_A}_{\text{because } N_A + N_B = N}$$

$$\Delta S^{mix,config} = -kN\left[\frac{N_A}{N} \ln X_A + \frac{N_B}{N} \ln X_B\right]$$

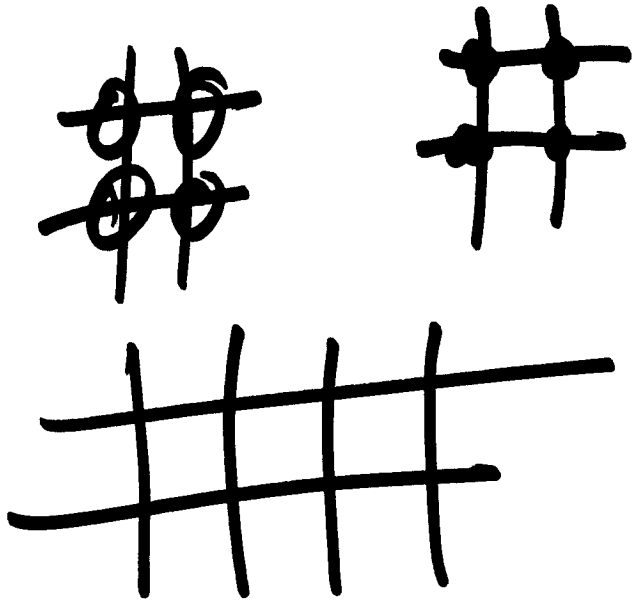
$$= -kN\left[X_A \ln X_A + X_B \ln X_B\right]$$

$$\Delta G^{mix} = -T\Delta S^{mix}$$

$$= +T.kN\left[X_A \ln X_A + X_B \ln X_B\right]$$

$$= T.R\left[X_A \ln X_A + X_B \ln X_B\right]$$

$$\underline{\Delta G^{mix} < 0.}$$



Regular solution model

$$\Delta G^{mix} = \Delta H^{mix} - T\underbrace{\Delta S^{mix}}_{\text{Configurational}}$$

$$-R\left[X_A \ln X_A + X_B \ln X_B\right]$$

$\Delta H^{mix} \neq 0$. $\Delta H^{mix} << 1$.

$$\Delta H^{mix} = \Omega X_A X_B = \Omega(1-X_B)X_B$$

$$\Omega = N_a z \varepsilon$$

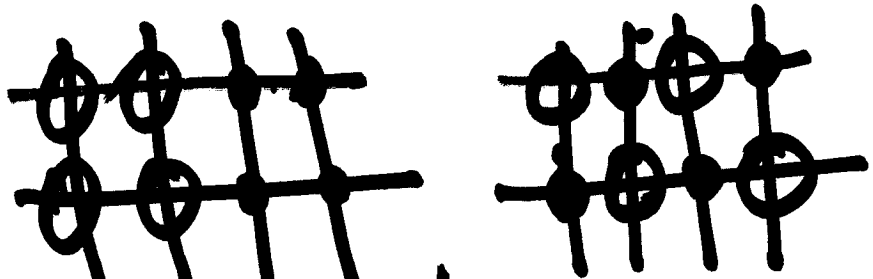
$$\varepsilon = E_{AB} - \frac{1}{2}(E_{AA} + E_{BB})$$

$$\Omega = N_a z \varepsilon$$

$$\Delta A_{mix} = \Omega X_A (1 - X_A)$$

$$\Delta G^{mix} = \Delta H^{mix} - T\Delta S^{mix}$$

$$= \Omega X_A (1 - X_A) + RT\left(X_A \ln X_A + (1 - X_A) \ln (1 - X_A)\right)$$



Ordered.

Immiscible/Phaseseparated.