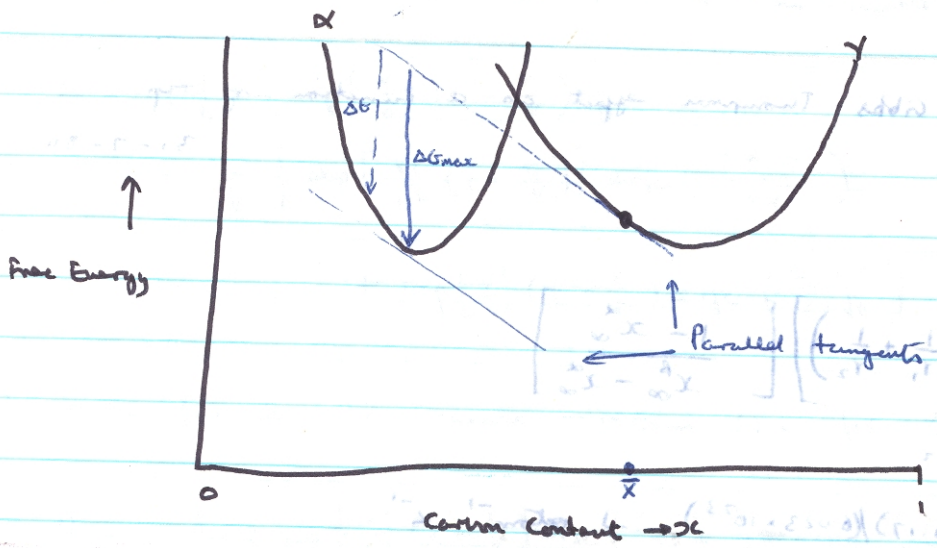
The Free Energy associated with Nucleation

2-8-80



Equation of tangent to γ curve at $x_\gamma = \bar{x}$ is

$$F = (1-x)\left\{F^{0\gamma}_{Fe} + RT \ln a^{\gamma}_{Fe}\{1-\bar{x}\}\right\} + x\left[F^{0\gamma}_{C} + RT \ln a^{\gamma}_{C}\{\bar{x}\}\right] \quad (A)$$

where $a\{\bar{x}\}$ = activity evaluated for mole fraction x

∴ ~~ΔG_{max} =~~ In general ∴

$$\Delta G = (1-x)\left[F^{0\alpha}_{Fe} + RT \ln a^{\alpha}_{Fe}\{1-x\}\right] + x\left[F^{0\alpha}_{C} + RT \ln a^{\alpha}_{C}\{x\}\right]$$
$$- (1-x)\left[F^{0\gamma}_{Fe} + RT \ln a^{\gamma}_{Fe}\{1-\bar{x}\}\right] - x\left[F^{0\gamma}_{C} + RT \ln a^{\gamma}_{C}\{\bar{x}\}\right]$$
$$= (1-x)\Delta F^{\gamma-\alpha}_{Fe} + (1-x)RT \ln \frac{a^{\alpha}_{Fe}\{1-x\}}{a^{\gamma}_{Fe}\{1-\bar{x}\}} + x\,RT \ln \frac{a^{\alpha}_{C}\{x\}}{a^{\gamma}_{C}\{\bar{x}\}} \quad (B)$$

For ΔG_{max}, the parallelism of tangents requires that

$$\left[F^{0\gamma}_{Fe} + RT \ln a^{\gamma}_{Fe}\{1-\bar{x}\}\right] - \left[F^{0\gamma}_{C} + RT \ln a^{\gamma}_{C}\{\bar{x}\}\right]$$

$$= \left[F^{0\alpha}_{Fe} + RT \ln a^{\alpha}_{Fe}\{1-x\}\right] - \left[F^{0\alpha}_{C} + RT \ln a^{\alpha}_{C}\{x\}\right]$$

or $$\Delta F^{\gamma-\alpha}_{Fe} + RT \ln \frac{a^{\alpha}_{Fe}\{1-x\}}{a^{\gamma}_{Fe}\{1-\bar{x}\}} - RT \ln \frac{a^{\alpha}_{C}\{x\}}{a^{\gamma}_{C}\{\bar{x}\}} = 0 \quad \ldots\ldots \quad (C)$$

Solving (B) and (C) simultaneously we get

$$\Delta G_{max} = RT \ln \frac{a^{\alpha}_{C}\{x\}}{a^{\gamma}_{C}\{\bar{x}\}}$$

To get a value of ΔG_{max} we have to solve (C) iteratively for x^{α}_{max}, substitute this into (B)