B10704007
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Thermodynamics of Materials II   Homework#5

$$1\ atm = 760\ mmHg = 1.01 \times 10^5\ N\ m^{-2}, R = 8.314\ J\ mol\ K^{-1}$$

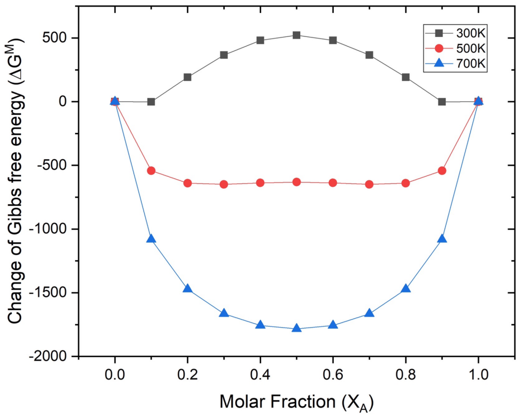
1 The change of Gibbs free energy of the A-B solution obeys the following equation:

$$\Delta G^M = RT(X_A \ln X_A + X_B \ln X_B) + 9000 X_A X_B$$

1.1 Plot the curves of ΔG^M $vs. X_A$ at 300 K, 500 K, and 700 K.

1.2 Get the expressions of $\Delta \bar{G}_A^M$ and $\Delta \bar{G}_B^M$.

1.1



1.2 By $\bar{M}_A = M + X_B \frac{dM}{dX_A} = M + (1-X_A)\frac{dM}{dX_A}$, $\bar{M}_B = M + X_A \frac{dM}{dX_B} = M - X_A \frac{dM}{dX_A}$

$\Delta G^M = RT(X_A \ln X_A + (1-X_A)\ln(1-X_A)) + 9000 X_A(1-X_A) = RT(X_A \ln X_A + \ln(1-X_A) - X_A \ln(1-X_A)) + 9000X_A - 9000X_A^2$

$\frac{d\Delta G^M}{dX_A} = RT(\ln X_A + 1 - \frac{1}{1-X_A} - \ln(1-X_A) + \frac{X_A}{(1-X_A)}) + 9000 - 18000X_A = RT(\ln \frac{X_A}{1-X_A}) + 9000 - 18000X_A$

$\therefore \Delta \bar{G}_A^M = RT(X_A \ln X_A + \ln(1-X_A) - X_A \ln(1-X_A)) + 9000X_A - 9000X_A^2 + (1-X_A)[RT(\ln \frac{X_A}{1-X_A}) + 9000 - 18000X_A]$

$= RT(\cancel{X_A \ln X_A} + \ln(1-X_A) - \cancel{X_A \ln(1-X_A)}) + \cancel{9000X_A} - 9000X_A^2 + RT(\ln \frac{X_A}{1-X_A}) + 9000 - 18000X_A - \cancel{X_A RT \ln \frac{X_A}{1-X_A}} - \cancel{9000X_A}$ $+18000X_A^2$

$= RT \ln X_A + 9000(X_A^2 - 2X_A + 1)$

$= RT \ln X_A + 9000(1-X_A)^2$

$\Delta \bar{G}_B^M = RT(X_A \ln X_A + \ln(1-X_A) - X_A \ln(1-X_A)) + 9000X_A - 9000X_A^2 - X_A[RT(\ln \frac{X_A}{1-X_A}) + 9000 - 18000X_A]$

$= \cancel{RT X_A \ln \frac{X_A}{1-X_A}} + RT \ln(1-X_A) + \cancel{9000X_A} - 9000X_A^2 - \cancel{RTX_A \ln \frac{X_A}{1-X_A}} - \cancel{9000X_A} + 18000X_A^2$

$= RT[\ln(1-X_A)] + 9000X_A^2$ #

2 The A-B solution shows the change of the molar enthalpy of the mix in the below figure.

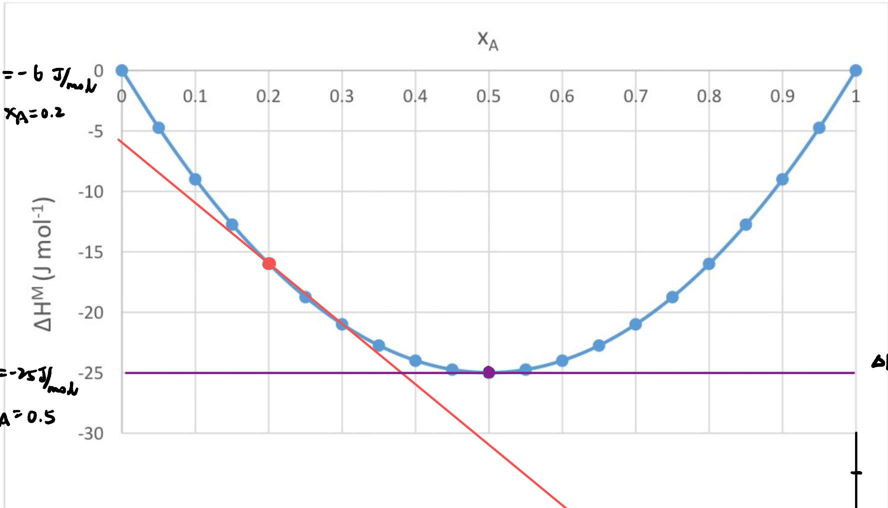
2.1 Get $\Delta\bar{H}_A$ and $\Delta\bar{H}_B$ at $X_A = 0.2, 0.5,$ and 0.8 using the method of intercepts (作圖截距法).

2.2 This curve is followed by $\Delta H_A^M = 100X_A^2 - 100X_A$. Determine $\Delta\bar{H}_A$ and $\Delta\bar{H}_B$ at $X_A = 0.2, 0.5,$ and 0.8, by using Gibbs–Duhem equation (整體求部分法)

2.3 Give the reasons if the answers of Q2.1 are different from the answers of Q2.2.

2.1

$\Delta\bar{H}_B = -6$ J/mol at $X_A = 0.2$ ①



$\Delta\bar{H}_B = -25$ J/mol at $X_A = 0.5$ ②

$\Delta\bar{H}_A = -25$ J/mol at $X_A = 0.5$ ②

$\Delta\bar{H}_A = -70$ J/mol at $X_A = 0.2$ ①

③ By Symmetry of the function,

$\Delta\bar{H}_A = -6$ J/mol at $X_A = 0.8$

$\Delta\bar{H}_B = -70$ J/mol at $X_A = 0.8$

2.2 $\Delta\bar{H}^M = 100X_A^2 - 100X_A$, $\dfrac{d\Delta\bar{H}^M}{dX_A} = 200X_A - 100$

$$\Delta\bar{H}_A = \Delta\bar{H}^M + (1-X_A)\frac{d\Delta\bar{H}^M}{dX_A} = 100X_A^2 - 100X_A + (1-X_A)(200X_A - 100)$$

$$= 100(X_A^2 - X_A + 2X_A - 1 - 2X_A^2 + X_A) = 100(-X_A^2 + 2X_A - 1) = -100(1-X_A)^2$$

$$\Delta\bar{H}_B = \Delta\bar{H}^M - X_A\frac{d\Delta\bar{H}^M}{dX_A} = 100X_A^2 - 100X_A - 200X_A^2 + 100X_A = -100X_A^2$$

	$X_A=0.2$	$X_A=0.5$	$X_A=0.8$
$\Delta\bar{H}_A$	-64	-25	-4
$\Delta\bar{H}_B$	-4	-25	-64

(unit J/mol) #

2.3 Because the line is drawn by people, the error exists when we are drawing the tangent line. Hence, the answer is different.