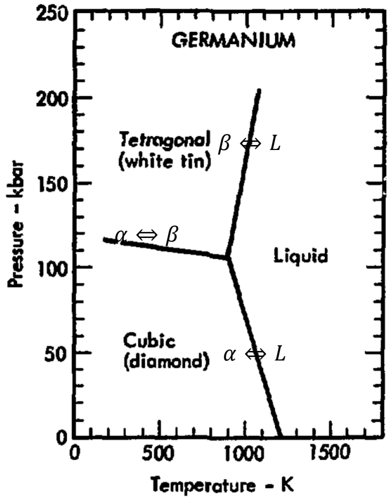
# MSE 103 Midterm 1 solutions

## Question 1

### Part A

Mark Asta 3/5/2016 11:59 AM

**Comment [1]:** Rubric: take off one point for each wrong two-phase label, and one point off each for wrong triple point temperature or pressure.



At triple point, T = 900 K and Pressure = 105 kbar

### Part B(i)

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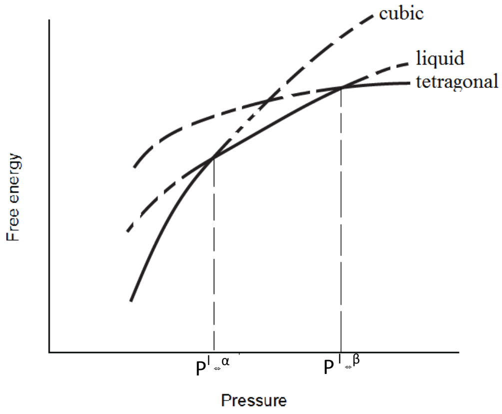
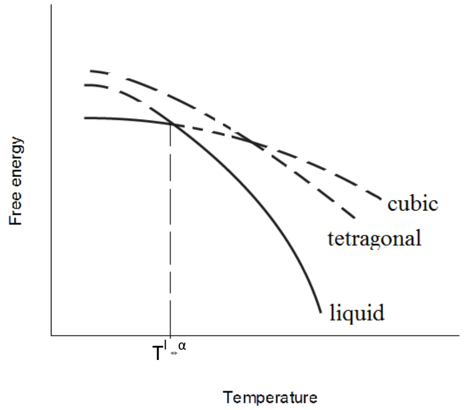
**Comment [2]:** Rubric: -2 if any of the curves have negative slopes, -1 if any of the curves have positive curvature, -2 if they don't have the right sequence of stable phases, -1 if any of the transition pressures are not labeled, --1 if the metastable cubic <-> tetragonal transition does not appear from the crossing of the curves.



## Part B(ii)



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**Comment [3]:** Rubric: -2 if any of the curves have positive slopes, -1 if any of the curves have positive curvature, -2 if they don't have the right sequence of stable phases, -1 if any of the transition temperature is not labeled, -1 if the slope of the tetragonal phase is not more negative than the cubic, -1 if liquid does not have the most negative slope.

## Part C(i)

Clausius-Clapeyron Relation:

$$\frac{dP^{\alpha\to L}}{dT} = \frac{\Delta\bar{S}^{\alpha\to L}}{\Delta\bar{V}^{\alpha\to L}} = \frac{\Delta\bar{H}^{\alpha\to L}}{T\Delta\bar{V}^{\alpha\to L}}$$

$\Delta\bar{H}^{\alpha\to L} = \frac{dP^{\alpha\Leftrightarrow L}}{dT} * T\Delta\bar{V}^{\alpha\to L}$ = -0.342 kBar $K^{-1}$* 900 K * -0.76 $cm^3$ $mol^{-1}$ * 100 J $cm^{-3}$ $kBar^{-1}$ = 23390 J $mol^{-1}$ = 23.39 kJ $mol^{-1}$

$\Delta\bar{S}^{\alpha\to L} = \frac{\Delta\bar{H}^{\alpha\to L}}{T}$ = 23390 J $mol^{-1}$ / 900 K = 25.99 J $mol^{-1}$ $K^{-1}$

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**Comment [4]:** Rubric: 6 points for this part, 9 for the next. In this part, 2 points for CC equation written somewhere, and 4 points for correct calculation. -1 if they use wrong temperature. -1 if they put all numbers correct but enter wrong in calculator and get wrong final answer. -1 if any of the numbers on the rhs for the enthalpy calculation are wrong. -1 for wrong units. Note, they do not have to compute DSa->b to get full points.

## Part C(ii)

$$\Delta\bar{S}^{\alpha\to L} = \Delta\bar{S}^{\alpha\to\beta} + \Delta\bar{S}^{\beta\to L}$$

Similarly, $\Delta\bar{V}^{\alpha\to L} = \Delta\bar{V}^{\alpha\to\beta} + \Delta\bar{V}^{\beta\to L}$

$\frac{dP^{\beta\to L}}{dT} = \frac{\Delta\bar{S}^{\beta\to L}}{\Delta\bar{V}^{\beta\to L}} = \frac{\Delta\bar{S}^{\alpha\to L}-\Delta\bar{S}^{\alpha\to\beta}}{\Delta\bar{V}^{\alpha\to L}-\Delta\bar{V}^{\alpha\to\beta}} = \frac{25.99-\Delta\bar{S}^{\alpha\to\beta}}{-0.76-\Delta\bar{V}^{\alpha\to\beta}}$ = 0.521 kBar $K^{-1}$ * 100 J $cm^{-3}$ $kBar^{-1}$ = 52.1 J $cm^{-3}$ $K^{-1}$ (Equation 1)

$\frac{dP^{\alpha\to\beta}}{dT} = \frac{\Delta\bar{S}^{\alpha\to\beta}}{\Delta\bar{V}^{\alpha\to\beta}}$ = -0.015 kBar $K^{-1}$ * 100 J $cm^{-3}$ $kBar^{-1}$ = -1.5 J $cm^{-3}$ $K^{-1}$ (Equation 2)

Solving for $\Delta\bar{S}^{\alpha\to\beta}$ using equations 1 and 2, we obtain:

**Mark Asta 2/24/2016 1:19 PM**

**Comment [5]:**
Rubric: 9 points for this one. 3 points for the first parts relating the alpha->beta values with the alpha->liquid and beta->liquid. 2 points for relevant CC equation. 2 points for right substitutions to get to right form to solve. 2 points for right answer with right units.

$\Delta\bar{S}^{\alpha\to\beta}$ = 1.835 J mol$^{-1}$ K$^{-1}$ and $\Delta\bar{V}^{\alpha\to\beta}$ = -1.224 cm$^3$/mole

## Question 2

### Part A

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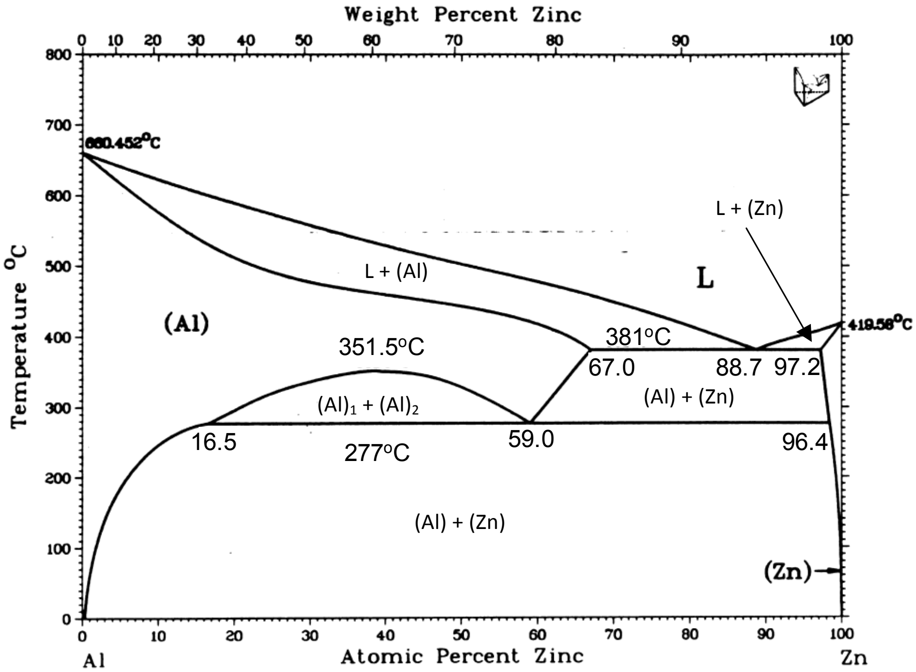
**Comment [6]:** Rubric: +1 for all correct 2-phase equilibria up to a maximum of +4 points. +1 for correct eutectic temperature.



Temperature of eutectic invariant equilibrium = 381˚C

### Part B

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**Comment [7]:** Rubric: 3 points for correctly identifying the right phases. 3 points for right compositions of the phases. 4 points for setting up lever rule and correctly solving for the phase fractions.

(Al) and (Zn) are the phases present.

Composition of (Al) = 0.645

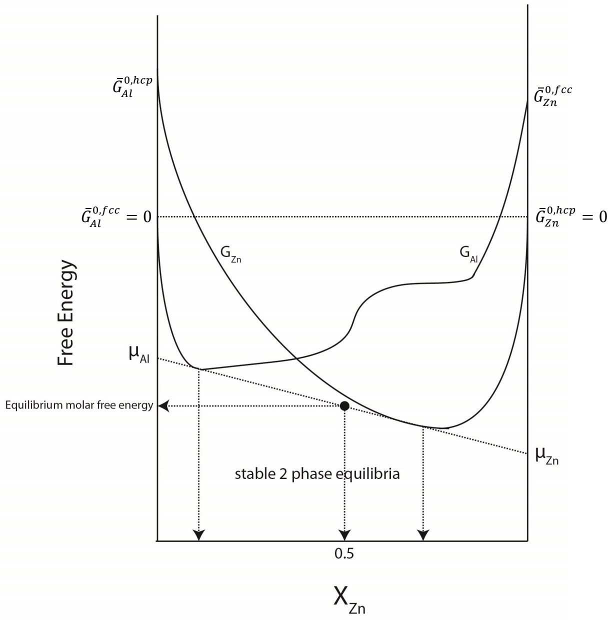
Composition of (Zn) = 0.975

Using lever rule,

Fraction of (Al) = (0.975-0.8)/(0.975-0.645) = 0.5303

Fraction of (Zn) = (0.8-0.645)/(0.975-0.645) = 0.4697

## Part C



## Part D

At 277°C, (Zn) is present with composition 0.964. Since the alloy at x=0.5 is within the monotectic equilibria, the chemical potential of all coexisting phases $(Al_1)$, $(Al_2)$ and (Zn) all have the same value for the Zn chemical potential ($\mu_{Zn}$). Therefore, the partial pressure for Zn in a vapor in equilibrium with all three phases will be the same as that calculated for (Zn).

For ideal solution, $a_{zn} = X_{Zn}$

So, $a_{zn} = 0.964$

Partial pressure = 0.964 * (6.1 * $10^{-7}$) = 5.880 x $10^{-7}$ atm

## Part E(i)

For the hcp (Zn) phase we can use Raoult's law to write,

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**Comment [8]:**
Rubric:
1 point for each endpoint (G0 values) correctly labeled. 4 points total.

1 points if the G curves start out with infinite slopes at the endpoints.

4 points for wiggle in G curve for (Al)

4 points for correct common tangent and compositions of the common tangents labeled.

4 points for method of intercepts and chemical potentials labeled.

3 point for correct chord construction to give the equilibrium free energy for x=0.5

-4 if the (Zn) phase has a wiggle in free energy given that we said it was ideal.

-3 if they do not put G_Al^0,fcc and G_Zn^0,hcp at zero.

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**Comment [9]:** Rubric:
5 points for identifying the activity of (Zn) using ideal solution

5 points for realizing that the (Zn) phase at 0.964 should be used to get the partial pressure even though x=0.5.

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**Comment [10]:** Rubric:
Part (i) = 14 points
Part (ii) = 3 points
Part (iii) = 3 points

For part (i):
+4 for activity of Zn being correct, including using Raoult's law and right composition
+4 for equating chemical potentials
+3 for rearranging the chemical potential equality equation and using the information about Ghcp-Gfcc.
+3 for correctly doing the math to get the right answer
For part (ii):
1 for correct definition for gamma
1 for identifying right value of x_Zn
1 for right math

Part (iii)
1 for right answer
2 for explanation

$a_{Zn}^{hcp} = X_{Zn}^{hcp} = 0.972$

Further, we know that in each phase (fcc and hcp) we can write:

$\mu_{Zn}^{fcc} = \bar{G}_{Zn}^{0,fcc} + RT \ln a_{Zn}^{fcc}$

$\mu_{Zn}^{hcp} = \bar{G}_{Zn}^{0,hcp} + RT \ln a_{Zn}^{hcp}$

At equilibrium, $\mu_{Zn}^{fcc} = \mu_{Zn}^{hcp}$

$\bar{G}_{Zn}^{0,fcc} + RT \ln a_{Zn}^{fcc} = \bar{G}_{Zn}^{0,hcp} + RT \ln a_{Zn}^{hcp}$

$\bar{G}_{Zn}^{0,fcc} - \bar{G}_{Zn}^{0,hcp} = RT \ln a_{Zn}^{hcp} - RT \ln a_{Zn}^{fcc}$

$1000 \text{ J mole}^{-1} = 8.314 \text{ J mole}^{-1} \text{ K}^{-1} * (381+273.15) \text{ K} * \ln (0.972 / a_{Zn}^{fcc})$

$a_{Zn}^{fcc} = 0.8087$

Part E(ii)

$a_{Zn}^{fcc} = \gamma_{Zn}^{fcc} X_{Zn}^{fcc}$

$X_{Zn}^{fcc} = 0.67$

Thus, $0.8087 = \gamma_{Zn}^{fcc} * 0.67$

$\gamma_{Zn}^{fcc} = 1.207$

Part E(iii)

$G^{xs}$ must be positive. This is because the activity coefficient is greater than one, implying that the chemical potential is larger than it would be for an ideal solution.  This implies that the excess contribution to G is positive.