MM209 Programming Assignment (Report)

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Group members:

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P7) Write a program which will generate phase diagram for Al_2O_3-Cr_2O_3 isomorphous system. Assume ideal solution for both solid and liquid phases.

- **Assumptions:**
  1. Solid and liquid phases form ideal solutions (Given) i.e., ideal solution model and complete miscibility in solid and liquid phases can be assumed.
  2. Total Pressure = 1atm
  3. Phase diagram is the 2D representation with composition of solutions (mol fraction (X)) along x axis and Temperature (in Kelvin) along y axis.
  4. The delC_p for pure solid ⇆ liquid eqm is 0 J/K/mol.

- **Methodology/Principle used for solving the above problem theoretically:**
  - Since the system is isomorphous (Given), delH_{mix} = 0 Joules/mol for the solution. The solid and liquid phases follow ideal model solution. This is why, this system gives the most ideal and simplest phase diagram as shown in the graph below.
  - The delG0 for pure liquid ⇆ solid eqm is zero only at the melting temperature of pure solid. In a two-component system, equilibrium can be achieved at any temperature between the melting temperatures of two pure solids.
  - The equations below explain that at any Temp (T) between $T_{melting}$ of pure solids, equilibrium between solid and liquid can be achieved which results in different compositions of solid phase and liquid phase at T.
  - Consider melting of pure solids as given by equations below

$Cr_2O_{3\,(s)} \leftrightharpoons Cr_2O_{3(l)}$ -(i)

$Al_2O_{3\,(s)} \leftrightharpoons Al_2O_{3\,(l)}$ - (ii)

delC_p = 0 J/K/mol (for above equilibrium equations)

$T_{melting}$ = del $H0_{melting}$/ del $S0_{melting}$

Given the values of del H0 and del S0, we can obtain del G0 for melting of pure solid as below:

$$\text{del } G0_{Melting,\, Cr2O3} = \text{del } H0_{Melting,\, Cr2O3} - T\,(\text{del } H0_{Melting,\, Cr2O3} / T_{melting,\, Cr2O3}) \quad \text{– (iii)}$$

$$\text{del } G0_{Melting,\, Al2O3} = \text{del } H0_{Melting,\, Al2O3} - T\,(\text{del } H0_{Melting,\, Al2O3} / T_{melting,\, Al2O3}) \quad \text{- (iv)}$$

In a two-component system, del G0 of melting is given by equations below:

$$\text{del } G_1 = \text{del } G0_{Melting,\, Cr2O3} + RT\ln(a_{Cr2O3(l)}/ a_{Cr2O3(s)}) \text{ for eqn(i)}$$

since, the liquid solution and solid solution both are ideal and P_T is 1 atm we can write

$a_{Cr2O3(s)}=X_{Cr2O3(s)}$

$a_{Cr2O3(l)} = X_{Cr2O3(l)}$

At equilibrium del G = 0; this gives us the following equation;

$$\text{del } G_1 = \text{del } G0_{Melting,\, Cr2O3} + RT\ln(X_{Cr2O3(l)}/ X_{Cr2O3(s)}) = 0 \quad \text{-(v)}$$

Similarly, using

$X_{Al2O3(s)} + X_{Cr2O3(s)} = 1$

$X_{Al2O3(l)} + XCr_{2O3(l)} = 1$

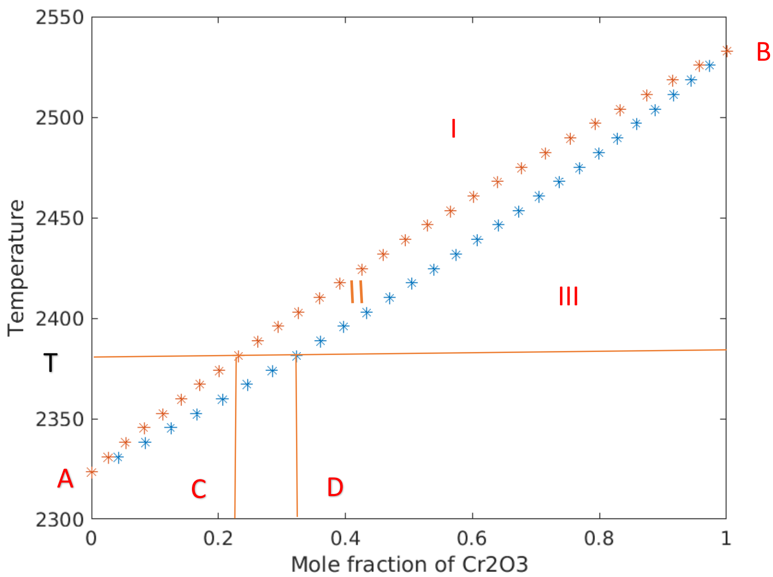
we obtain;

$$\text{del } G_2 = \text{del } G0_{\text{Melting, Al2O3}} + RT\ln((1-X_{Cr2O3(l)})/(1-X_{Cr2O3(s)})) = 0 \qquad \text{-(vi)}$$

- At any temp (**T**), we can obtain del $G0_{melting}$ for both components using eqn(iii) and eqn (iv), which is used to get different equilibrium compositions ($X_{Cr2O3(l)}$) of the solid ($X_{Cr2O3(s)}$) and liquid solutions respectively from equation (v) and (vi).
- This makes us possible to get the phase diagram for such system as shown below.

- **Phase diagram plot: (methodology used to code is in the README file)**
  (We have used MATLAB to obtain the phase diagram plot.)

  - Numerical Data used includes
    1. del $H0_{melting\ (Al2O3)}$ = 107500 J/mol
    2. del $H0_{melting\ (Cr2O3)}$ = 117400 J/mol
    3. $T_{melting\ (Al2O3)\ (s)}$ = 2324 K
    4. $T_{melting\ (Cr2O3)\ (s)}$ = 2358 K
  - Source (references) for numerical data:
    - INTRODUCTION TO THE THERMODYNAMICS OF MATERIALS (FOURTH EDITION) - David R. Gaskell
      Table – A5; Page no. 587 data for del$H0_{melting}$ of Al_2O_3, Problem 10.3; Page no. 302 data for $T_{melting}$ of $Al_2O_{3\ (s)}$ and $Cr_2O_{3(s)}$.
    - Gaskell solutions Text Notes Problem 10.3 data for del $H0_{melting}$ of Cr_2O_3.



- **Explanations of the plots and results:**
  - Region I is a single-phase region (Liquid) with degrees of freedom, F=1.
  - Region II is a two phases region (Liquid ⇆ Solid) with F=2.
  - Region III is a single-phase region with F=1.
  - Line separating regions I and II is called liquidus and line separating regions II and III is called solidus.
  - Point **A** on y axis is $T_{Melting}$ of Al_2O_3 and point **B** is $T_{Melting}$ of Cr_2O_3

- The plot shows mol fraction of Cr_2O_3 along x axis and temperature (in Kelvin) along y axis.
- At temp **T** as shown by the red horizontal line, we obtain different equilibrium compositions for solid and liquid phase respectively.
- Eqm value of $X_{Cr_2O_3\,(l)}$ i.e., (liquid eqm composition) is given by point **C** on x axis and $X_{Cr_2O_3(s)}$ i.e., (solid eqm composition) is given by point **D** on x axis.
- Therefore, at Temp **T** if we fix the eqm composition of solid solution we obtain a fixed eqm composition for liquid solution and vice-versa.

- **Contributions made by each member:**
  - Each member contributed equally in developing the code and worked on getting the methodology right for the problem.
  - Sahensu Soni (190110078) researched and obtained the numerical data needed.
  - Rhythm Shah (190110074) created the final code and obtained the plots.
  - Neha Parasharam Jadhav (190110053) worked on the explanations of the results, plots and made the final report.

- **GitHub link to the project:**
  https://github.com/rhythm-shah/MM209CodingAssignment