Final Project – CME 572: Advanced Thermodynamics of Materials

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Total Points: 120

Due Date: May 1, 2022 by 11:59 pm

This is an open-book open-note final project. Your final exam questions will be based on the report you prepare for this final project.

- For this project, you need to perform phase diagram calculations using the ThermoCalc software. Please refer to the "ThermoCalc" tab on Blackboard for instructions on using the software.
- You are to do your own work, but you can discuss the technical aspects of the ThermoCalc software with others.
- Please make sure to show all your work and state all your assumptions in the report. Submit all your input files and plots with your report.
- Submit your report as a single pdf file to Blackboard. Submission of multiple files is not accepted.
- If you have any question, email me at `sarakad@uic.edu`.
- The final report is due by Monday May 1st 11:59 pm.

Take the following steps and prepare a final report. The final report should be a single pdf file.

Define the Binary System

Select a binary system of your interest. Please follow the instructions on how to select your system on the share Google document at `https://docs.google.com/document/d/1IDl79GrpEpKk3EvS1EAw6cR2Myzz4LzxeuVVAzDWSZo/edit?usp=sharing`.
A sample project for Ni-Mn with the necessary calculation steps in ThermoCalc is available on the "ThermoCalc" tab on Blackboard.

Calculation of the Phase Diagram (50 points)

Calculate the binary phase diagram for your system in the T-X space. A suggested temperature range is from room temperature to 2000-3000 K.

(a) (10 points) Illustrates the step by step calculation process in ThermoCalc in your report. Take screen snapshots of each step in the process (e.g., a snapshot of you system definition step)and embed them in your report. Please do not include separate files for this. You should explain each step with any specific assumption above each screen shot in a few sentences.

(b) (10 points) Finally, show the phase diagram plot. Use the label feature in ThermoCalc to specify all the single phase regions and two phase regions.

(c) (15 points) Specify 1) the highest melting point (in K) and the corresponding composition X (in mole% or mass%), 2) the lowest melting point (in K) and the corresponding composition X, 3) the melting point (in K) for unary systems. Show all of them over the phase diagram plot as well.

(d) (5 points) If there is any intermediate phase in your system, specify them.

(e) (10 points) What is the stable phase for the corresponding unary systems (reference states) at room temperature?

Calculation of the Gibbs energy (50 points)

Calculate the Gibbs energy curves for your system (G-X curves).

(a) Illustrates the step by step calculation process in ThermoCalc in your report for the followings.

(b) (10 points) Show the G-X curves at the highest melting point (T=highest melting point). Show on the plot the lowest Gibbs curve and the corresponding phases. Make sure to specify the phases associated with the common tangents to the curves (if any).

(c) (10 points) Show the G-X curves at the lowest melting point. (T=lowest melting point). Show on the plot the lowest Gibbs curve and the corresponding phases. Make sure to specify the phases associated with the common tangents to the curves (if any).

(d) (10 points) Show the G-X curves at 200 K above the room temperature. (T=498 K). Show on the plot the lowest Gibbs curve and the corresponding phases. Make sure to specify the phases associated with the common tangents to the curves (if any).

(e) (10 points) Show the G-X curves at the room temperature. (T=298 K). Show on the plot the lowest Gibbs curve and the corresponding phases. Make sure to specify the phases associated with the common tangents to the curves (if any).

(f) (10 points) Show the G-X curves at a temperature at which there exist either an intermediate phase or a two phase coexistence. Show on the plot the lowest Gibbs curve and the corresponding phases. Make sure to specify the phases associated with the common tangents to the curves (if any).

Calculation of the Activity (20 points)

Calculate the activity (referred to a phase) for your system (a-X curves).

(a) Illustrates the step by step calculation process in ThermoCalc in your report for the followings.

(b) (10 points) Show the a-X curves for the activity of both components at 200 K above the room temperature and for all the relevant phases at that temperature. Specify whether the system exhibit a negative or a positive departure from the ideal behavior at each phase.

(c) (10 points) Show the a-X curves for the activity of both components at the lowest melting point and for all the relevant phases at that temperature. Specify whether the system exhibit a negative or a positive departure from the ideal behavior at each phase.