

3.020, Spring 2021

Thermodynamics of Materials

Problem Set 6

Massachusetts Institute of Technology
Department of Materials Science and Engineering

Due April 16, 2021 at 10am EDT

We encourage you to work in groups. If you do so, please note the names of your groupmates on the first page of your solutions.

Remember to clearly present your solutions, including intermediate steps. Failure to show your work may result in reduced credit. Sloppy presentation may result in reduced credit.

Thermo 6.1: The lever rule [3 pts]

Derive the lever rule for binary systems

Thermo 6.2: Exploring the Ag-Cu system, part II [12 pts]

On problem set 5 you explored the Ag-Cu system using Thermo-Calc. Now we'll pick up where we left off.

- [1 pts] Use the phase diagram and the lever rule to estimate the equilibrium state (phase fractions, and compositions of each phase) of the system at $P = 1$ atm, $T = 1000$ K, and an overall composition of 20% Cu.
- [3 pts] Plot the molar Gibbs free energy Cu(ss) and Ag(ss) phases at $P = 1$ atm, $T = 1000$ K, using X_{Cu} as the x-axis. Both curves should appear on the same plot; be sure to label them clearly. Indicate which parts of the curves make sense, for instance by using hashmarks to show which part of the curves are not to be believed (*e.g.* the data may not be available).
- [2 pts] Draw a common-tangent construction on your plot from part (b), use it to graphically estimate the equilibrium state of the system, and compare to your estimate from part (a).
- [2 pts] Graphically estimate the chemical potentials of both components in both phases at the equilibrium conditions considered in part (a).
- [2 pts] Estimate the partial molar Gibbs free energy of mixing of both components in both phases at the equilibrium conditions considered in part (a).
- [2 pts] Calculate the activity of both components in both phases at the equilibrium conditions considered in part (a).

Thermo 6.3: Stability and instability [6 pts]

Show that binary phases with negative curvature $\frac{d^2\Delta G_{\text{mix}}}{dX^2} < 0$ are unstable with respect to small composition fluctuations, with constant overall composition.

Thermo 6.4: Frog and toad aren't friends [9 pts]

(After DeHoff problem 8.5) The system Froggium (Fr) - Toadium (Td) is found to have partial molar heat of mixing for Froggium given by:

$$\Delta \bar{H}_{\text{Fr}} = 12500X_{\text{Fr}}X_{\text{Td}}^2 \text{ (J/mol)}$$

- [3 pts] Calculate the heat of mixing ΔH_{mix} for this system
- [3 pts] Assume this system behaves as a regular solution. Will this system exhibit spinodal decomposition? Why or why not? *Hint: Consider the temperature-dependence of ΔG_{mix}*
- [3 pts] Plot the Gibbs free energy of mixing of this system at 240 K. If there are any common tangents, draw them (by hand is fine), and indicate the resulting two-phase region(s).

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