ME-351 THERMODYNAMICS AND ENERGETICS II

SPRING 2025

QUESTION 1

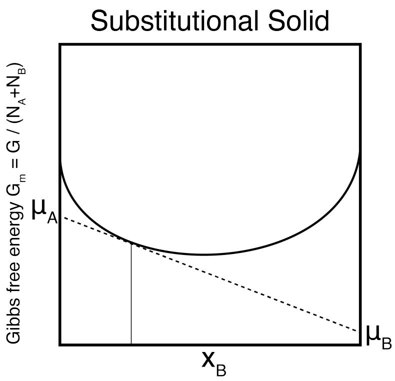

Figure 1

Dilute concentrations of impurities such as hydrogen, carbon, oxygen etc. typically occupy *interstitial* sites of the crystal structure in metallic alloys. Interstitial sites refer to the space or "holes" between atoms in a crystal structure. Molar quantities in interstitial solids are normalized somewhat differently as compared to substitutional solids, which we discussed in class. Let the number of atoms of element A and B be denoted N_A and N_B respectively. For an interstitial solid, where A is the "host" (A could be a metal such as titanium, zirconium, iron etc.) and B is the interstitial specie (B could be elements such as hydrogen, oxygen, carbon etc.), the molar Gibbs free energy and concentration are defined as:

$$G_m = \frac{G}{N_A}$$

$$x = \frac{N_B}{N_A}$$

1. Derive the graphical construction shown in fig. 1, for the chemical potential of B in an intersitial solid.
2. Schematically sketch the chemical potential of B in an interstitial solid for materials with free energy curves shown in fig. 2

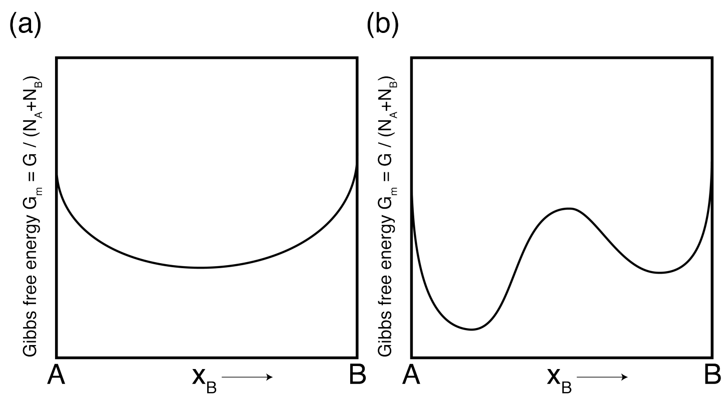

Figure 2

QUESTION 2

Consider the phase diagram shown in fig. 3. Sketch the free energies for all phases marked in the phase diagram at the temperatures marked T_1, T_2, T_3, and T_4. Clearly indicate the equilibrium compositions of all phases at each temperature. Mark these compositions on the phase diagram.

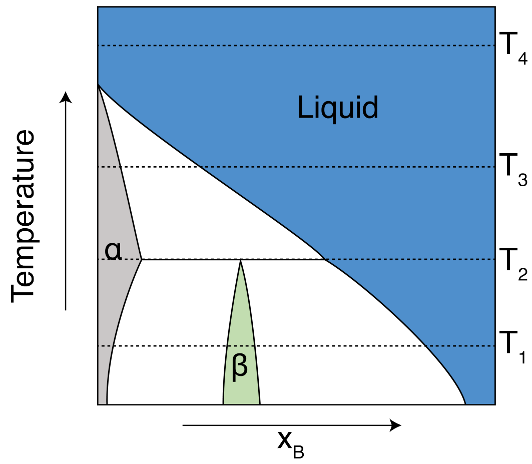

Figure 3

QUESTION 3

An alloy system is found to have phases with free energies as shown fig. 4. Sketch the temperature-composition phase diagram for this material system. As indicated in the *empty* phase diagram: $T_1 < T_2 < T_3 < T_4$

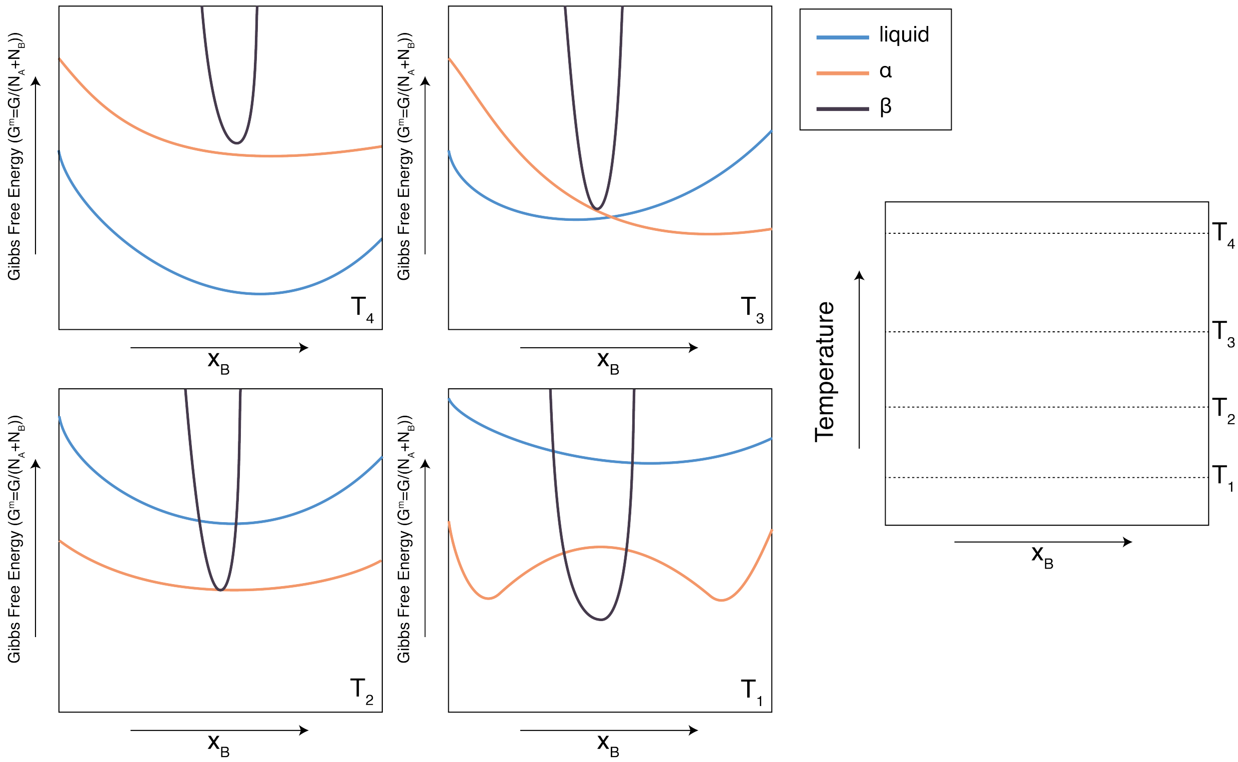

Figure 4

QUESTION 4

A binary mixture of two chemical species (denoted A and B) is found to have the following free energy function:

$$G^m(x,T) = \Omega x(1-x) + k_B T(x\log(x) + (1-x)\log(1-x))$$

where $G^m = \frac{G}{N}$ is the molar Gibbs free energy of the solid, $x = N_B/N$ is the mole fraction of specie B, T is the temperature, $N = N_A + N_B$ is the total number of atoms, Ω is a positive number and $k_B = 8.617 \times 10^{-5}$eV/K/atom is Boltzmanns constant.

1. Derive an expression for the enthalpy ($H^m(x,T) = H/N$) and entropy ($S^m(x,T) = S/N$) of the mixture
2. Express the chemical potential of B in terms of x, Ω, T, k_B
3. Assuming $\Omega = 0.1eV/atom$, plot G^m, H^m and S^m as a function of composition at $T = 400K$ and $T = 800K$ using your favorite plotting program.
4. Analytically, show that the free energy is at an extremum when $x = \frac{1}{2}$ for any positive value of Ω
5. Using the second derivative of the free energy with respect to composition, find the temperature above which the free energy at $x = \frac{1}{2}$ is always a minimum. Notice that above this temperature, the free energy is convex, while below this temperature the free energy will contain concave regions.
6. Sketch the $T - x$ phase diagram of the binary mixture.