MSE-483 ADVANCED PHASE TRANSFORMATIONS

FALL 2025

QUESTION 1

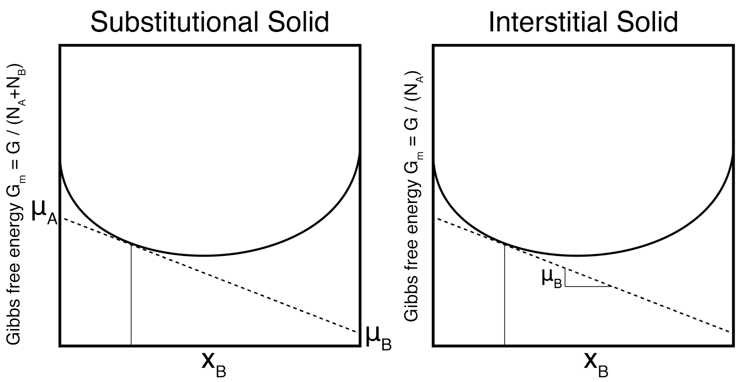

Figure 1

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

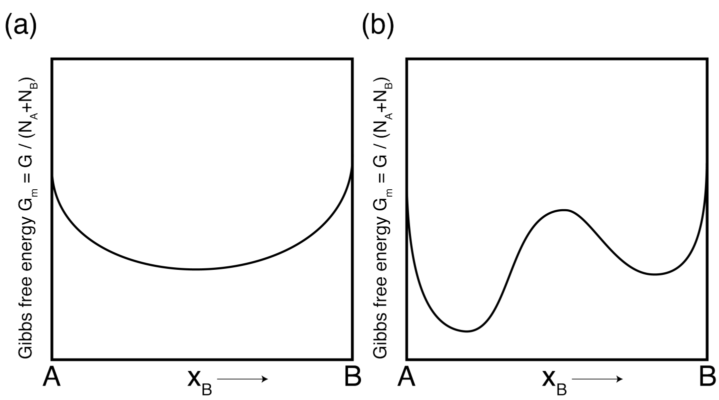

Figure 2

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.

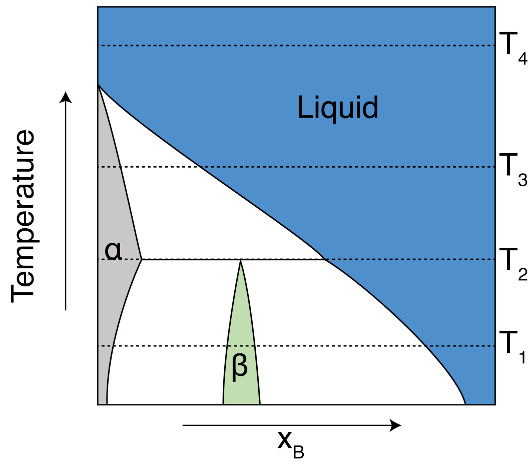

Figure 3

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: $T_1 < T_2 < T_3 < T_4$

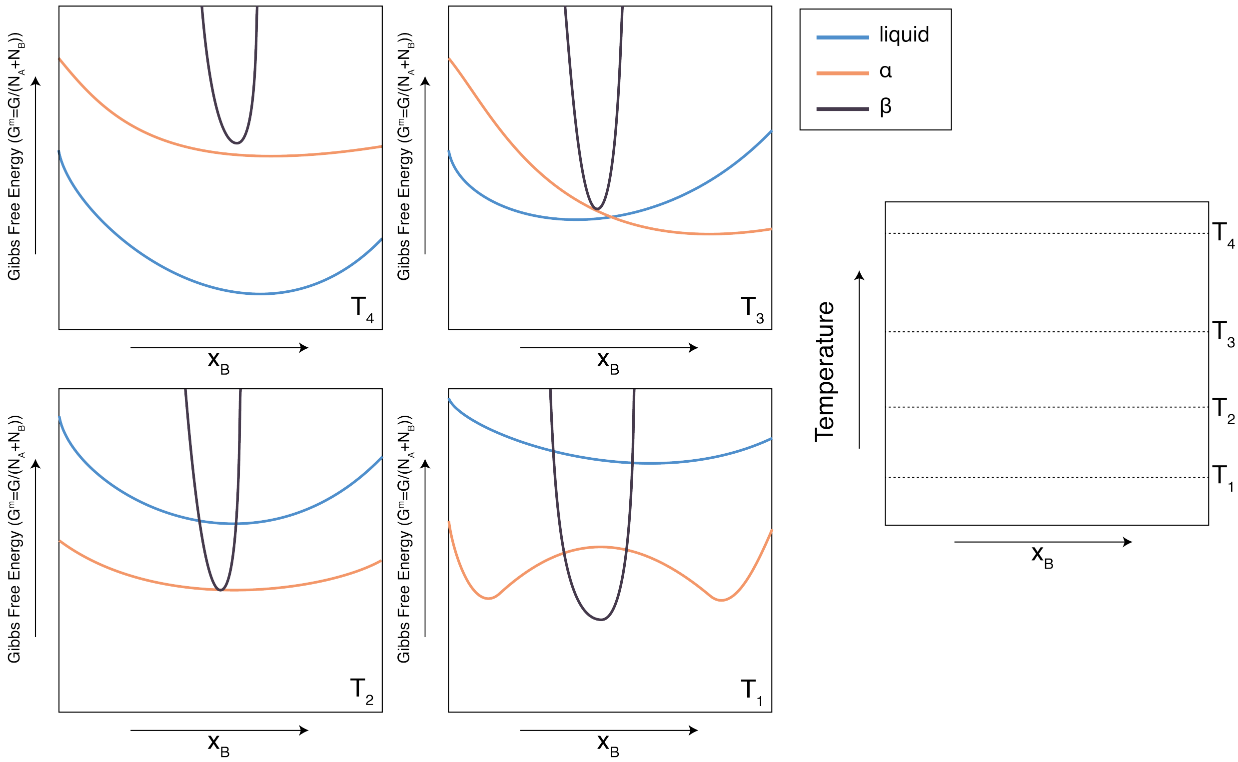

Figure 4

QUESTION 4

A rod made of a single element is subject to a gradient in temperature and chemical potential. It is placed within an electric field that induces a gradient of the electrical potential within the material. The chemical, thermal and electric driving forces are denoted $\nabla\mu$, $\frac{\nabla T}{T}$ and $\nabla\phi$ respectively.

1. Write down the generalized flux equations for the material under these conditions. Give each coupling coefficient a unique label such as L_{11} (coefficient coupling chemical flux of specie "1" to chemical potential of specie "1"), L_{1q} (coefficient coupling chemical flux of 1 to temperature gradient), L_{1Q} (coefficient coupling chemical flux to charge current) etc.
2. How many unique L coefficients are there in the coupled force-flux equations?
3. In the absence of chemical and thermal gradients, relate the L coefficients to the electrical conductivity (ρ) of the material
4. Based on the positive entropy generation postulate of irreversible thermodynamics, what is the sign of electrical conductivity?
5. Say that the material is an electrical insulator and diffusion of the chemical specie is extremely fast. A constant thermal gradient is imposed along the bar, while the electric field is removed. Derive an expression relating the thermal conductivity of the material to L_{qq}, L_{q1}, and L_{11}.

QUESTION 5

Consider a metallic rod of length L containing a uniform concentration of interstitial species dissolved within the metal. The rod is brought into contact with thermal reservoir at temperature of T_1 at one end and a temperature of T_2 at the other end. The temperatures of the reservoirs are such that $T_1 < T_2$.

1. Write down the equations that couple the thermal and compositional fluxes to the driving forces for heat and mass flux. You can assume that only the interstitial specie is mobile in the rod.
2. What conditions must be met by the L coefficients for the interstitial atoms to not diffuse due to the thermal gradient?
3. What conditions must the coupling constants meet for the interstitial atoms to diffuse towards the hotter end of the bar?

QUESTION 6

Consider a material containing a charged specie (such as Li^+) that is allowed to freely diffuse through it. A gradient in chemical and electric field is imposed on the material. Derive a flux relation for the charged specie as a function of the two driving forces : $\nabla\mu$ and $\nabla\phi$. Charge is constrained to be only transported by the charged specie. You can neglect any thermal gradients and chemical gradients of other chemical species in the material. The electrical charge per ion is q_1.
HINT: Re-derive an equation that relates the rate of entropy generation in the material starting from the fundamental equation of thermodynamics. Impose the constraint that $dq = q_1 dc$

QUESTION 7

The Fourier transform of a one-dimensional function is defined as :

$$\mathcal{F}\{c(x,t)\} = \tilde{c}(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} c(x,t) e^{ikx} dx$$

Show that $\mathcal{F}\{\frac{\partial^2 c}{\partial x^2} = -k^2 \tilde{c}(k,t)\}$ when $c(x = \pm\infty, t) = 0$ and $\frac{\partial c(x=\pm\infty,t)}{\partial x} = 0$