3.012 PS 6 **3.012**
Issued: 11.29.05 **Fall 2005**
Due: 12.9.05

STRUCTURE

1. **X-ray generation:** What is the minimum wavelength that X-rays emitted from a metal target can have, when the target is hit by electrons accelerated in a potential difference of 10 kV ? What will be the wavelength of the K_β radiation ? (Answer both questions for the case of a copper target, and that of a molybdenum target).

2. **Reciprocal lattice:** given a body-centered cubic lattice, with primitive vectors (-a/2, a/2, a/2), (a/2, -a/2, a/2), (a/2, a/2, -a/2), what will be its reciprocal lattice, and what will be the primitive vectors of the reciprocal lattice ?

3. **Diffraction:** suppose we have a one-dimensional line of atoms at a distance of 2 A from each other, and we have an incident X-ray beam of wavelength 1 A arriving at an angle of 70 degrees.

   a. At what angles, if any, will we see outgoing diffraction cones, and what will be their diffraction order (i.e. the difference in wavelengths between the spherical wave emitted by one scatterer, and the one emitted by the next scatterer) ? Draw a clear sketch of the system, of the incoming radiation, and of the outgoing cones. Consider all the diffraction cones that can be produced.
   b. Suppose now that we insert one atom in between every atom in this one-dimensional line; can you explain, in graphical terms, what will be the additional diffraction cones appearing ?

4. **Ewald construction:** what will be the wavelength needed to see a [001] reflected beam from the BCC crystal given in question 2 ?

5. **A Debye Scherrer experiment:** the following values for 2θ are measured in a powder diffraction experiment of a cubic crystal: 20.3, 23.6, 32.3, and 41.6 . What is the lattice parameter for the conventional unit cell of this system ? Can this crystal be BCC ? FCC ? Simple cubic? (The incident radiation corresponds to the K_α line of copper)

6. **Conductivity and symmetry:** let's consider the Hg-Ba-Cu superconducting oxide of Problem 3.25 (Allen-Thomas, p. 210).

   a. What is the point group symmetry of this material ?
   b. What could be a generator group (see p. 186) ?
   c. What will be the non-zero elements of the second-rank conductivity tensor relating the current to the applied field ? Name all the inequivalent elements as a, b, c…
   d. Suppose we apply a field E_0 in the [111] direction. What will be the resulting current ? What will be the angle between the current and the field ? [Beware: vectors and tensors are expressed in Cartesian coordinates, but the [111] direction is in crystallographic coordinates – i.e. as a function of the direct lattice vectors]

THERMODYNAMICS

1. **Building a binary phase diagram**. Given below are data for a binary system of two materials A and B. The two components form three phases: an ideal liquid solution, and two solid phases α and β that exhibit regular solution behavior. Use the given thermodynamic data to answer the questions below.

LIQUID PHASE:

$$\left(\mu_A^o\right)^L = -500 - 4.8T \frac{J}{mole}$$

$$\left(\mu_B^o\right)^L = -1{,}000 - 10T \frac{J}{mole}$$

(T is temperature in K)

ALPHA PHASE:

$$\left(\mu_A^o\right)^\alpha = -6000 \frac{J}{mole}$$

$$\left(\mu_B^o\right)^\alpha = -1{,}000 \frac{J}{mole}$$

Ω = 8,368 J/mole

BETA PHASE:

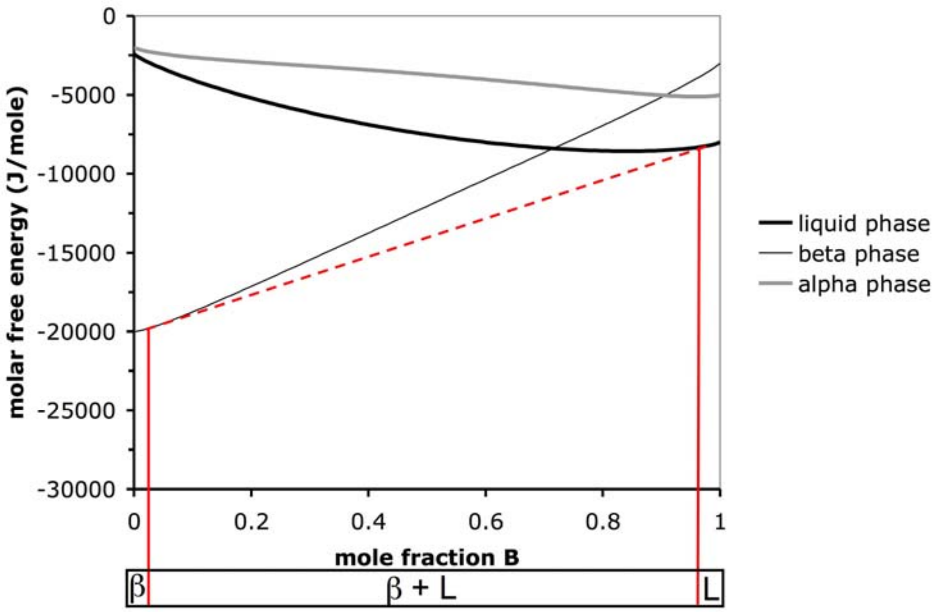
$$\left(\mu_A^o\right)^\beta = -4{,}000 - 1.09T \frac{J}{mole}$$

$$\left(\mu_B^o\right)^\beta = -13{,}552 - 2.09T \frac{J}{mole}$$

(T is temperature in K)

Ω = 7,000 J/mole

a. Plot the free energy of L, alpha, and beta phases (overlaid on one plot) vs. X_B at the following temperatures: 2000K, 1500K, 1000K, 925K, and 800K. For each plot, denote common tangents and drop vertical lines below the plot to a 'composition bar', as illustrated in the example plot below. For each graph, mark the stable phases as a function of X_B in the composition bar below the graph, as illustrated in the example.



b. Using the free energy curves prepared in part (a), construct a qualitatively correct phase diagram for this system in the temperature range 800K – 2000K. Mark the invariant points on the diagram with a filled circle.

2. **Analyzing stable equilibria with binary phase diagrams.** Shown below is the phase diagram for the binary system MgO-Al_2O_3 at P = 1 atm. Use the diagram to answer the questions below.

   a. At T = 1750°C (broken line marked on diagram), what is the makeup of the system (what phases are present, what is the phase fraction of each phase, and what is the composition for each phase) at X_{Al2O3} = 0.2 and X_{Al2O3} = 0.6?

   b. Mark the invariant points on the diagram and label what the type of each.

   c. Draw a qualitatively reasonable diagram of the molar free energy of each phase vs. X_{Al2O3} for T = 1750°C (overlay all of the curves on the same diagram). Mark the common tangents with a dashed line.

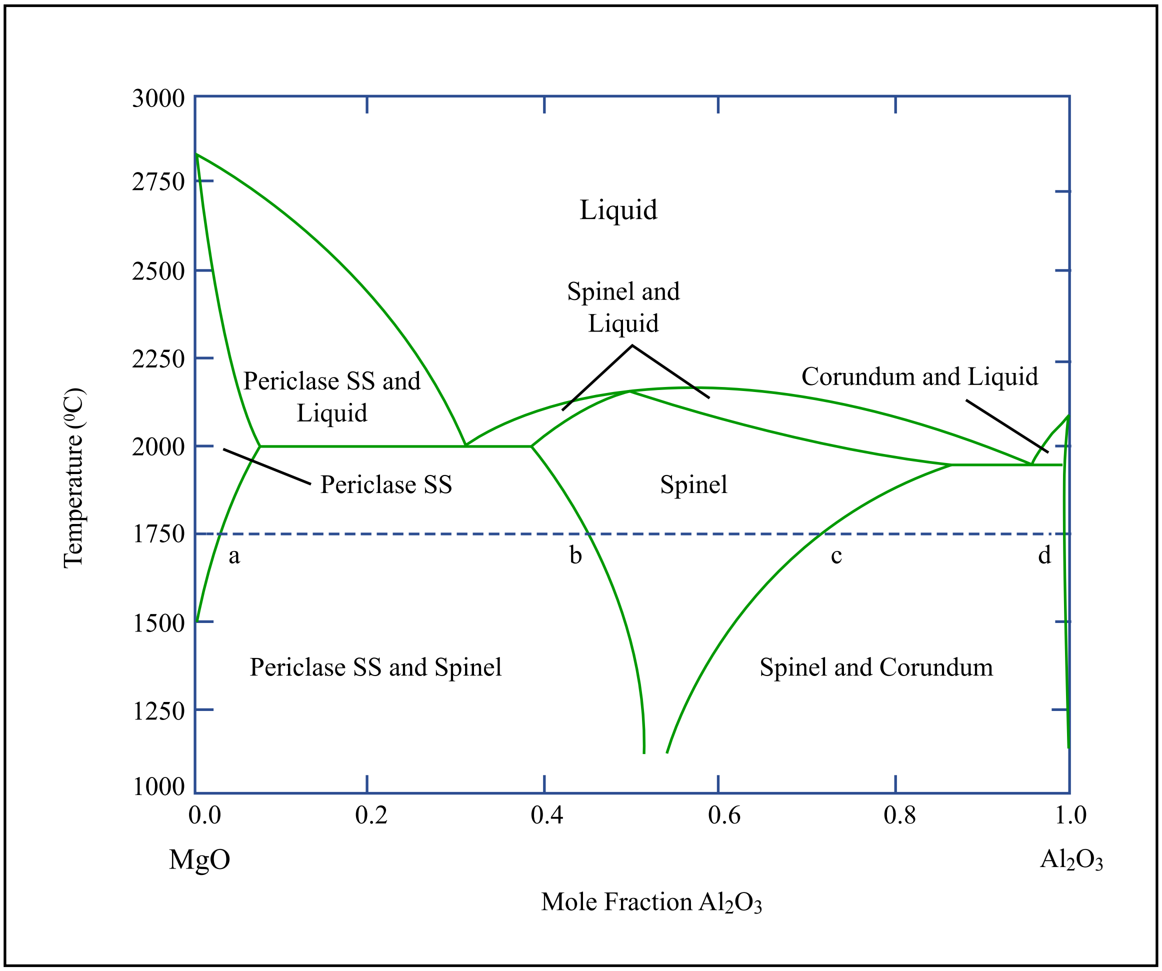
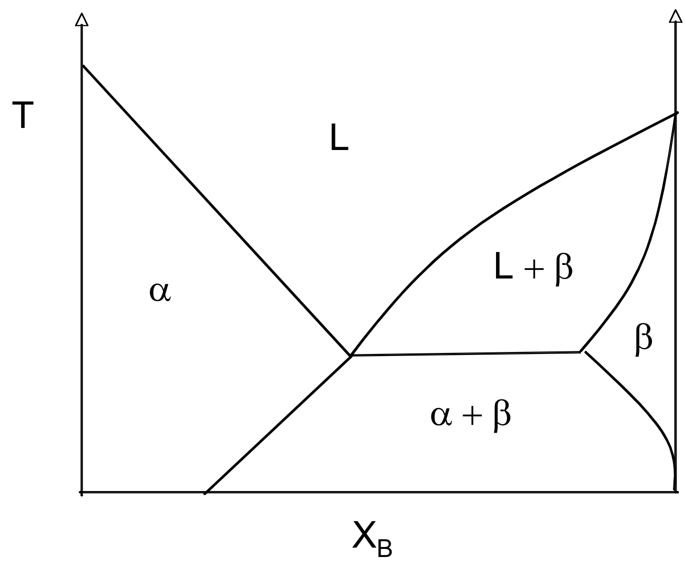


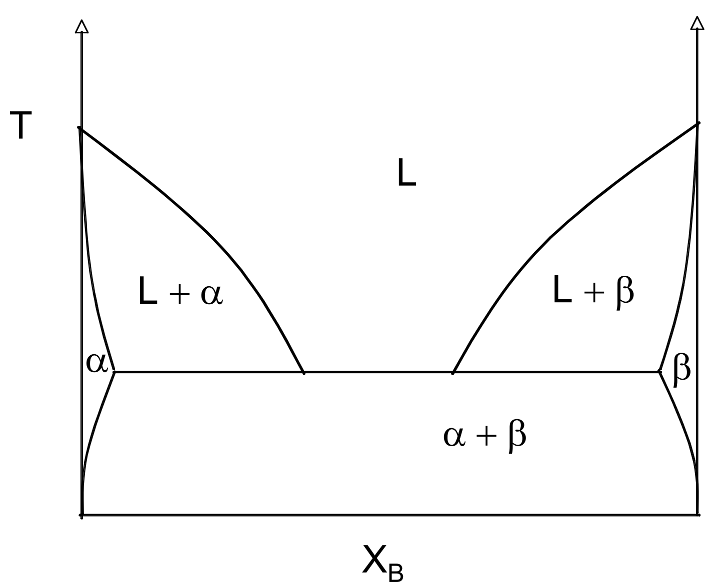
Figure by MIT OCW.

3. **The structure of phase diagrams is not arbitrary**. Given below are two hypothetical structures for binary phase diagrams. Using sketches of Gibbs free energy curves vs. composition and/or a few brief sentences, explain why each of the proposed phase diagram structures is impossible.

   a. A solid phase alpha has a continuous boundary with liquid and no intervening two-phase (α + L) region:



   b. A diagram with a broad boundary between liquid and phase-separated α/β solids:



4. **Metastable and unstable systems**. Consider a regular solution with the following thermodynamic parameters:

$$\mu_A^o = -2{,}000 \frac{J}{mole}$$

$$\mu_B^o = -3{,}000 \frac{J}{mole}$$

$$\Omega = 8{,}500 \frac{J}{mole}$$

(Assume the standard state chemical potentials are approximately constant for this calculation.)

a. For a solution with a mole fraction B of 0.3 being cooled from elevated temperatures, at what temperature would phase separation first be observed (supposing the system is constantly re-equilibrating as the temperature is dropped)? *Hint: Your calculation is simplified by the fact that miscibility gap of simple regular solutions is symmetric about X_B = 0.5.*

b. The mode of phase separation in a system (nucleation and growth vs. spinodal decomposition) can be controlled by quenching (rapidly cooling) a system from a homogeneous high-temperature state to a temperature where one mode of phase separation or the other will be operable. What is the lowest temperature that this solution with a mole fraction B of 0.3 could be quenched to and still obtain spinodal decomposition?

5. **Peritectic phase diagrams**. Use the given phase diagram for the binary system of copper and cobalt to answer the questions below.

a. Draw a reasonable set of free energy curves for each phase of the Cu-Co system at 1400°C, the peritectic temperature of 1385°C, and just below the peritectic at 1350°C.

b. Suppose a solution with 50 mole% Cu were cooled to 1400°C and equilibrated, then further cooled to 1200°C. How much "primary" β-Co phase would be present in the final sample (mole fraction)? How much *total* β-Co phase would be present in the final sample (mole fraction)?

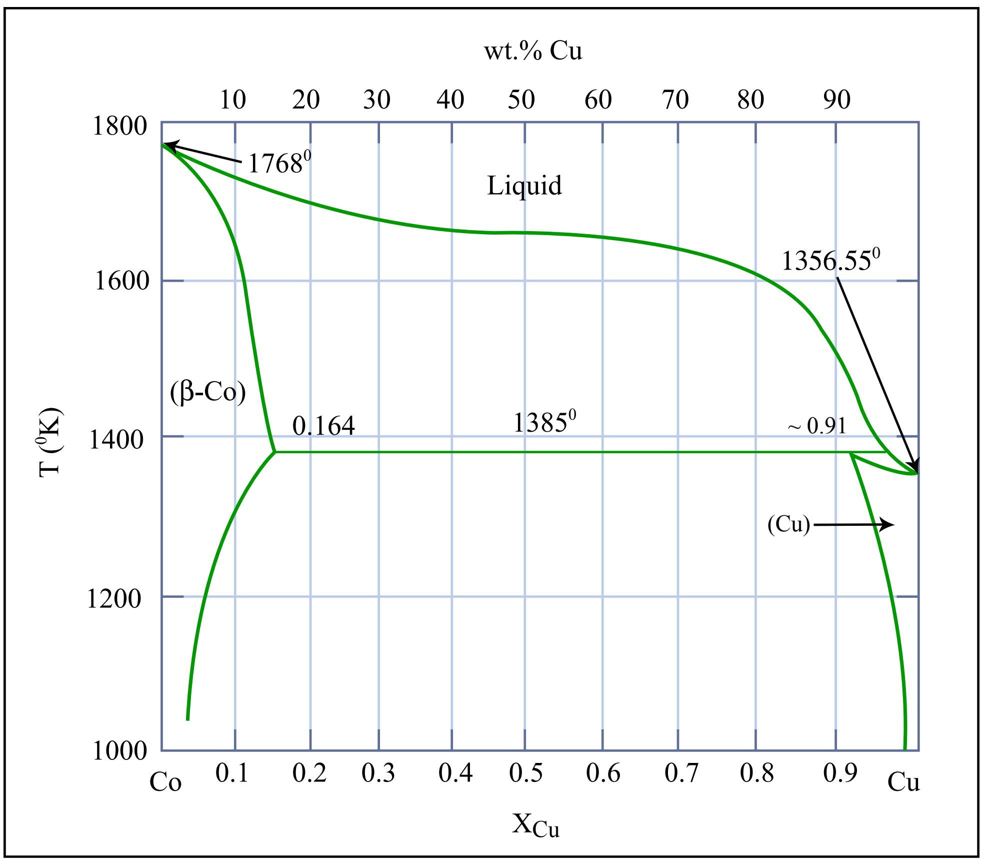


Figure by MIT OCW.