

Department of
MATERIALS SCIENCE AND ENGINEERING

Doctoral Written Exam

Core Areas:

**Materials Physics And Chemistry
Advanced Mechanical Behavior
Advanced Thermodynamics Of Materials
Kinetics and Phase Transformations
Structure Of Materials**

Thursday, May 20, 2010

Department of Materials Science and Engineering

DOCTORAL WRITTEN EXAM

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Your exam packet contains 3 questions from each core area for which you signed up, along with several answer sheets. A copy of the Table of Constants is included for your reference. **You must submit 2 questions from each core area you are taking for grading.** You will have 1 1/2 hours to complete each section. You can obtain extra answer sheets from the proctor, if needed. Please use the following procedure:

Write a four (4) digit code of your choice, and your name on the page provided. Use this code in place of your name to identify all answer sheets you submit for both days of the exam. Renee will keep the code information, sealed in an envelope, until after the exams are graded.

For each answer, use the question sheet as the first page of your answer. If additional pages are required, use the blank answer sheets provided. At the end of the examination, staple each question sheet and corresponding answer sheets for each question separately, put this instruction sheet on top of the questions you are turning in, and place them in one side of your exam folder. Place all other exam pages in the other side of your folder, and return everything to Renee if you finish before your time is up.

Please be sure to complete the information required on each page.

CODE NUMBER _____

CHECK THE QUESTIONS YOU WISH TO HAVE GRADED:

Materials Physics
And Chemistry:

1. _____

2. _____

3. _____

Advanced Mechanical
Behavior:

4. _____

5. _____

6. _____

Advanced Thermodynamics
Of Materials

7. _____

8. _____

9. _____

Kinetics and Phase
Transformations

10. _____

11. _____

12. _____

Structure of Materials

13. _____

14. _____

15. _____

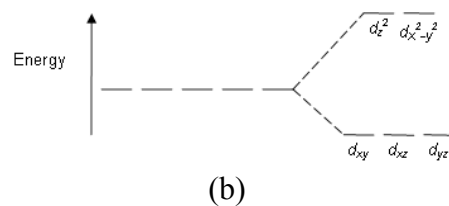
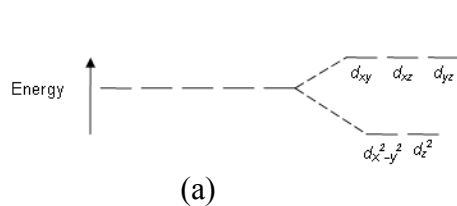
1.

BaTiO₃ at 25 °C is tetragonal with the lattice constants of $a = 3.992 \text{ \AA}$ and $c = 4.036 \text{ \AA}$. BaTiO₃ is a paraelectric for $T > T_c = 130^\circ\text{C}$ and has a spontaneous polarization of 0.26 C/m^2 at 25 °C.

- (a) Calculate the electric dipole moment p of the BaTiO₃ unit cell at 25 °C.
- (b) As temperature decreases, how does the polarization of BaTiO₃ change?
- (c) What is the total number of possible ferroelectric variants (domains) at room temperature?

2.

Figures shown below show the energy splitting of 3d orbital according to crystal field theory. Indicate which is in the tetrahedral configuration and which is in the octahedral configuration? Explain why?



3.

Consider a one-dimensional monatomic solid with N atoms and $N_L(V)$ vacancies at temperature $T > 0$ K. Show that the fractional vacancy concentration $n_v(T) = N_L(V)/N$ is given approximately by $n_v \approx \Delta/l_0 - \Delta a/a_0$. Here $l_0 = Na_0$ is the length of the solid at $T = 0$ K, and Δa is the change in the lattice constant.

4.

A plate of the epoxy reinforced unidirectional Kevlar 49 Fibers ($E_x = 76000$ ksi) is subject to stresses, $\sigma_x = 400$, $\sigma_y = 12$, $\tau_{xy} = 15$ MPa, for the usual coordinate system. Determine the in-plane strain, ϵ_x , ϵ_y and γ_{xy} .

5.

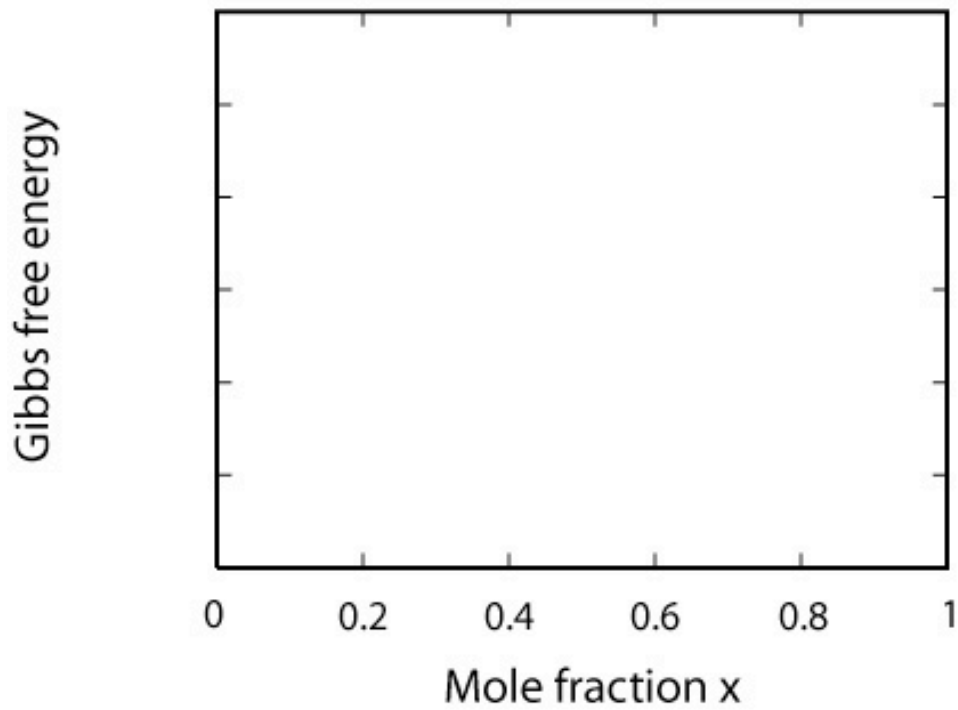
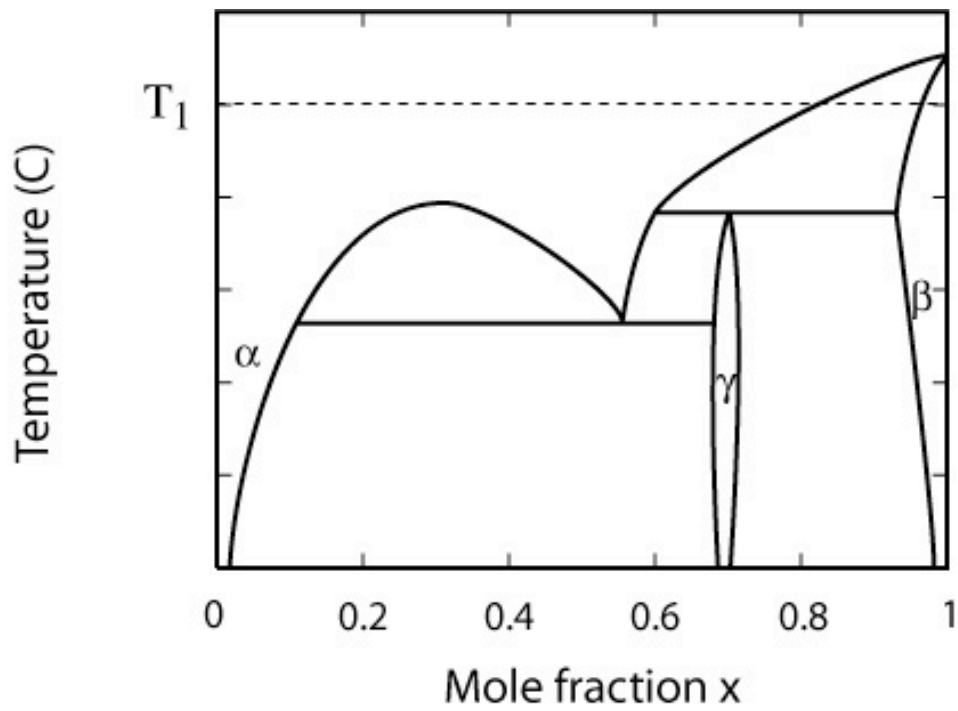
A cylindrical pressure vessel 10m long has closed ends a wall thickness of 5 mm and an inner diameter 3 m. The vessel is filled with gas to a pressure of 2 MPa. Determine the maximum normal stress and the maximum shear stress and orientation of the planes on which they act.

6.

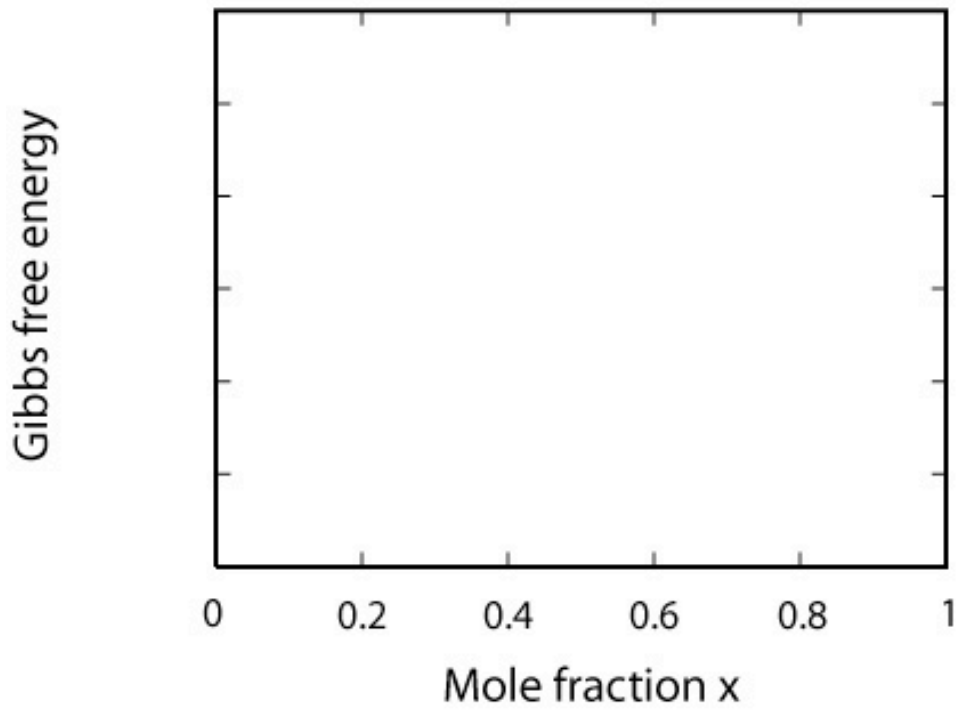
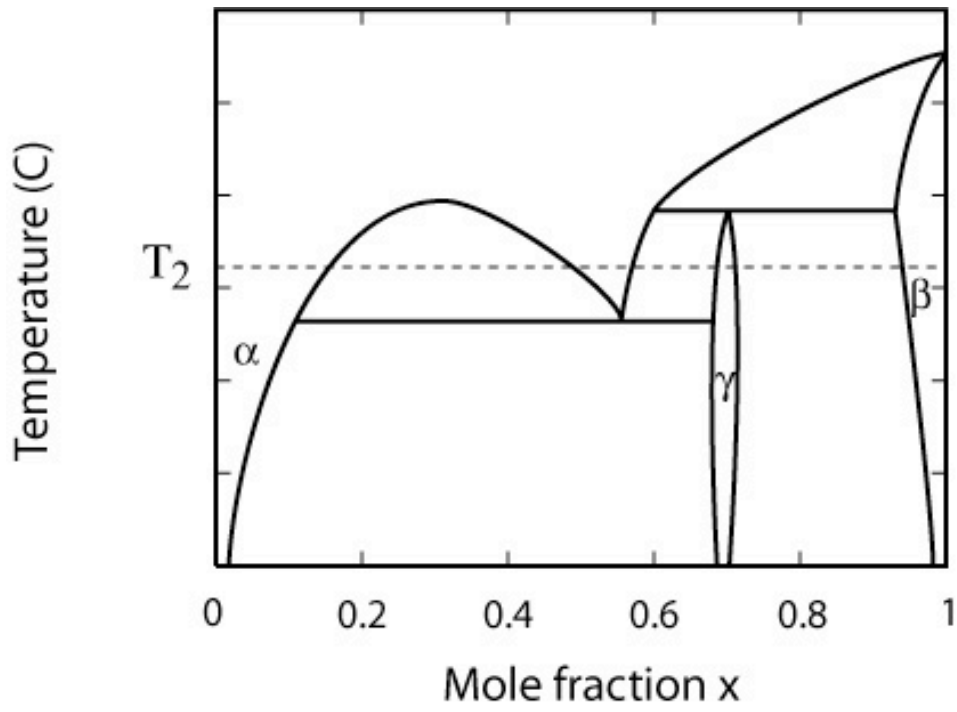
An engineering component made of the heat resisting Fe-Cr-Ni- Co alloy S-590 is subjected in service to a static stress of 200 MPa at a temperature of 600C. What creep-rupture life in days is expected?

7.

a) Schematically draw the free energies of the A-B alloy at temperature T_1 .



b) Schematically draw the free energies of the A-B alloy at temperature T_2 .

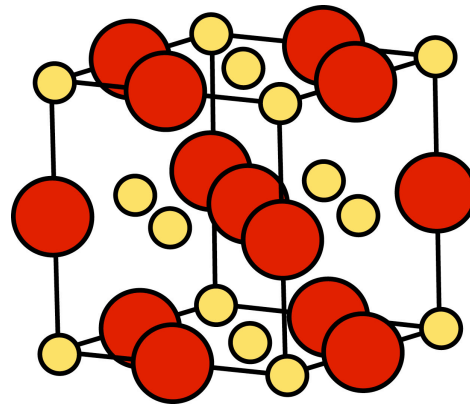
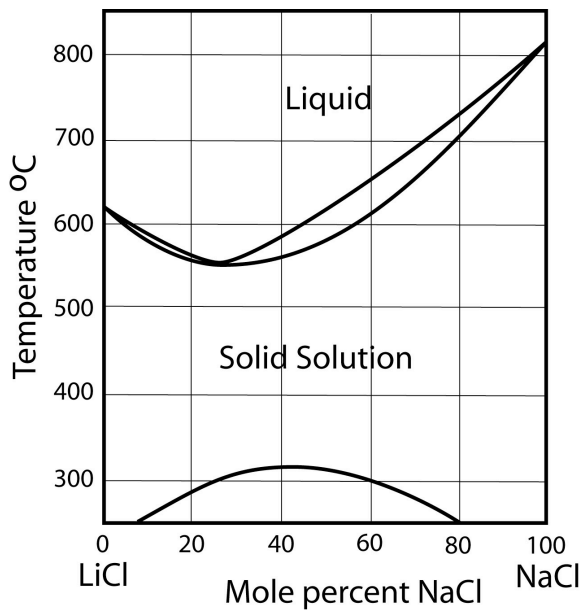


8.

Derive the equilibrium criteria for two-phase coexistence (between an α phase and a β phase) in a binary A-B alloy at constant temperature and pressure. The total number of A and B atoms, N_A and N_B , are constant.

9.

Below is the phase diagram for LiCl-NaCl, both of which have the rock salt crystal structure also illustrated below. The small atoms represent Li and Na (i.e. Li and Na mix on one of the sublattices) and the large atoms are Cl anions. The phase diagram exhibits miscibility gap below 314°C.



- Assuming a regular solution model is appropriate for describing the free energies of mixing in the solid solution, write down the regular solution model free energy for this system and explicitly write out how the regular solution parameter is related to atomic bond energies in the LiCl-NaCl system. Be specific about which bond energies matter and what species are interacting in the bond energies you write out.
- Is $\omega > 0$ or < 0 ? Rationalize the sign of ω on the basis of the information given.

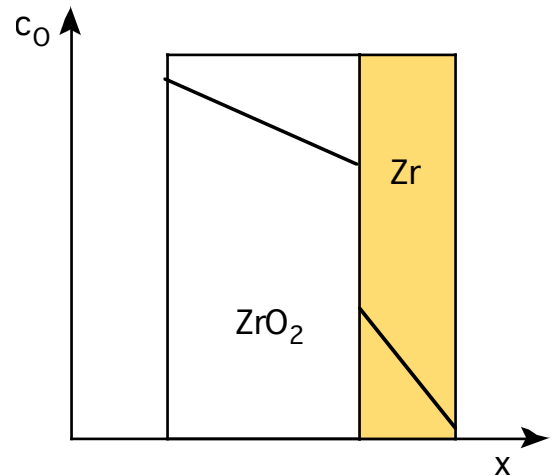
10.

Assume a thin foil of zirconium, heated to 1000K. On one side the foil is exposed to pure oxygen, on the other side to pure carbon monoxide (CO). The oxidation of Zr progresses as oxygen diffuses across the ZrO_2 layer. However, because Zr metal has a finite solubility for oxygen, the reaction at the ZrO_2/Zr interface is slowed down and comes to a halt before all Zr is oxidized.

a) Explain why.

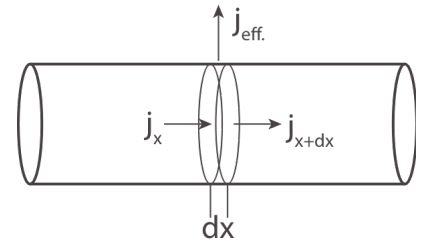
b) What are the relative thicknesses of the ZrO_2 and Zr layers after very long time. Assume that the gas compositions on either side do not change.

For your explanations refer to the adjacent schematic. The molecular weight of Zr is 91.22 g/mol, that of O is 16 g/mol. The density of ZrO_2 is 5.6 g/cm³ and that of Zr is 6.49 g/cm³. The concentration of oxygen in ZrO_2 at the ZrO_2 /gas interface is 1.08 times higher than at the ZrO_2/Zr interface. The maximum solubility of oxygen in Zr is 2.5 mol%. The equilibrium concentration of oxygen in Zr at the Zr/CO(gas) interface is zero. The diffusion coefficients of O in ZrO_2 and Zr at that temperature are $2.3 \cdot 10^{-7}$ and $6.5 \cdot 10^{-6}$ cm²/s respectively.



11.

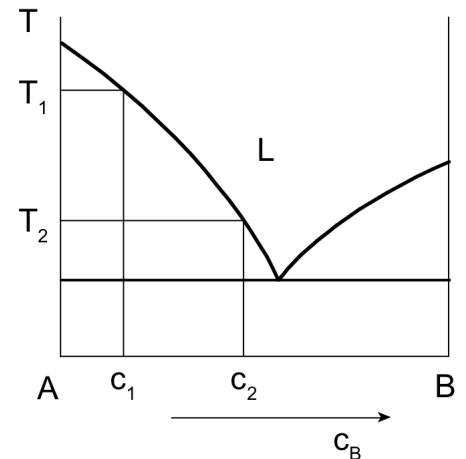
A hydrocarbon gas containing 1 mol-% N_2 impurities flows through a porous tube at 500 K. The pores in the tube wall are large enough to allow for the N_2 molecules to effuse, but they are too small to let the hydrocarbon molecules through. The total cross section of the pore orifices constitutes 0.01% of the total inside wall surface of the tube. The gas flow rate is $0.005 \text{ m}^3/\text{s}$.



- Derive the expression that gives the N_2 concentration in the gas as a function of the coordinate along the tube axis in flow direction. Given the small concentration of N_2 , ignore any changes in the density of the gas.
- Calculate the length of the tube needed to reduce the N_2 concentration to $1/32$ of its initial value. The molecular weight of $N_2 = 28 \text{ g/mol}$.

12.

Two elements A and B form a eutectic, as illustrated in the adjacent phase diagram. At first, an A-rich liquid mixture of A and B is held at temperature T_1 . Some pure A precipitates and remains in equilibrium with a liquid of composition c_1 . Subsequently, the system is quenched to temperature T_2 and held there again. Additional A precipitates as the liquid is depleted of component A. Assume that the interface between the liquid mixture and pure solid A remains planar throughout the process, no convection occurs in the liquid, and the growth of phase A progresses in one dimension only.



- Derive the expression that describes the thickness of the layer of solid A as a function of time. (If encounter the need to describe the concentration of a species as a function of time and location resulting from a diffusion process, it is sufficient you know the solution for this process; there is no need to derive it.)
- Calculate the thickness of the additional growth of A (since quenching it to T_2) at time $t = 1000$ s, knowing that the diffusion coefficient of A in the liquid is $6.8 \cdot 10^{-6}$ cm²/s, $c_1 = 0.02$ mol/cm³, and $c_2 = 0.05$ mol/cm³. The solubility of B in A is negligible.

13.

- a) What is the angle between $[100]$ and $[111]$ in a cubic system?
- b) What is the angle between (100) and (111) in a cubic system?
- c) What is the c/a ratio of the ideal hexagonal close packed (*hcp*) structure?
- d) Describe the procedure to measure the angle between two poles (p and q).

14.

How would you distinguish between the following imaging features within TEM? Why does your method work?

- a) Moiré fringes against wedge thickness fringes.
- b) Bend contours against dislocation arrays.
- c) Moiré fringes against dislocation arrays.

15.

Figure shown below is a phase diagram of two metals A and B that are partially soluble. Draw schematics to show the characteristics of x-ray diffraction patterns ($\vartheta-2\vartheta$) of the solid solutions at H, K, L, and M, respectively. Assuming the α phase has a f.c.c. structure, while the β phase has a b.c.c structure.

