

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**

Friday, January 27, 2011

Department of Materials Science and Engineering

DOCTORAL WRITTEN EXAM  
January 27, 2011

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 3 X 5 card 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. \_\_\_\_\_

**4.**

A block of pure Ni single crystal is loaded in uniaxial tension with a stress,  $\sigma_{xx}$ , equal to 100 MPa parallel to the  $\langle 100 \rangle$  direction.

Assume:

- C11 = 246.5 GPa
- C12 = 147.3 GPa
- C44 = 124.7 GPa
- S11 = 0.0073 GPa<sup>-1</sup>
- S12 = 0.0027 GPa<sup>-1</sup>
- S44 = 0.0080 GPa<sup>-1</sup>

For polycrystalline pure Ni

- E = 199.5 GPa
- G = 76.0 GPa
- $\nu = 0.312$

- a) Determine the elastic moduli in the  $\langle 100 \rangle$ ,  $\langle 110 \rangle$  and  $\langle 111 \rangle$  directions.
- b) Assuming that 100 MPa is well below the proportional limit determine the strains in the  $\langle 100 \rangle$ ,  $\langle 010 \rangle$  and  $\langle 001 \rangle$  directions.
- c) Now assume that the block is composed of polycrystalline Ni, determine the strains in the x, y and z directions and provide an explanation for the differences between the values in part b and c.

**5.**

An aluminum alloy consists of 3.3 volume percent of a hard, spherical phase in an FCC aluminum matrix. The precipitates are 20nm in diameter and are separated by a distance of 50 nm.

Assume:

$$E = 70 \text{ GPa}$$

$$G = 26.1 \text{ GPa}$$

$$\nu = 0.345$$

$$\text{Burger's Vector} = 0.286 \text{ nm}$$

Precipitates are arranged in a simple cubic arrangement

- a) Calculate the shear stress required to move a dislocation through the ductile FCC matrix.
- b) Heat treatment of the aluminum alloy increases the precipitate diameter to 50 nm. Calculate the stress required to move a dislocation through the FCC matrix. Show all assumptions.

6.

A mechanical structure made from an aluminum alloy is subjected to a cyclic stress of 75 MPa at an R Ratio of -1. The alloy's characteristics are:

$$E = 70 \text{ GPa}$$

$$G = 26.1 \text{ GPa}$$

$$\nu = 0.345$$

$$\text{Yield strength} = 700 \text{ MPa}$$

$$\text{Fatigue Strength Exponent, } b = -0.1$$

$$\text{Fatigue Strength Coefficient, } \sigma_f' = 600 \text{ MPa}$$

$$\text{Paris Law Constant, } c = 8 \times 10^{-11} \text{ mm/cycle}$$

$$\text{Paris law Exponent, } m = 3$$

$$K_Q = 80 \text{ MPa-m}^{1/2}$$

$$K_{IC} = 40 \text{ MPa-m}^{1/2}$$

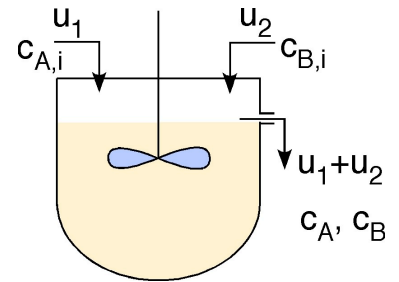
- a) Calculate the number of cycles at which a fatigue crack will initiate.
- b) During fatigue loading a crack 2mm in length is detected. Calculate the size of a crack that will cause catastrophic failure and the number of cycles that would elapse. For the purpose of this analysis, assume that the crack is in an infinite, homogeneous structure, loaded under plane strain conditions.

## Kinetics and Phase Transformations

Code \_\_\_\_\_

10.

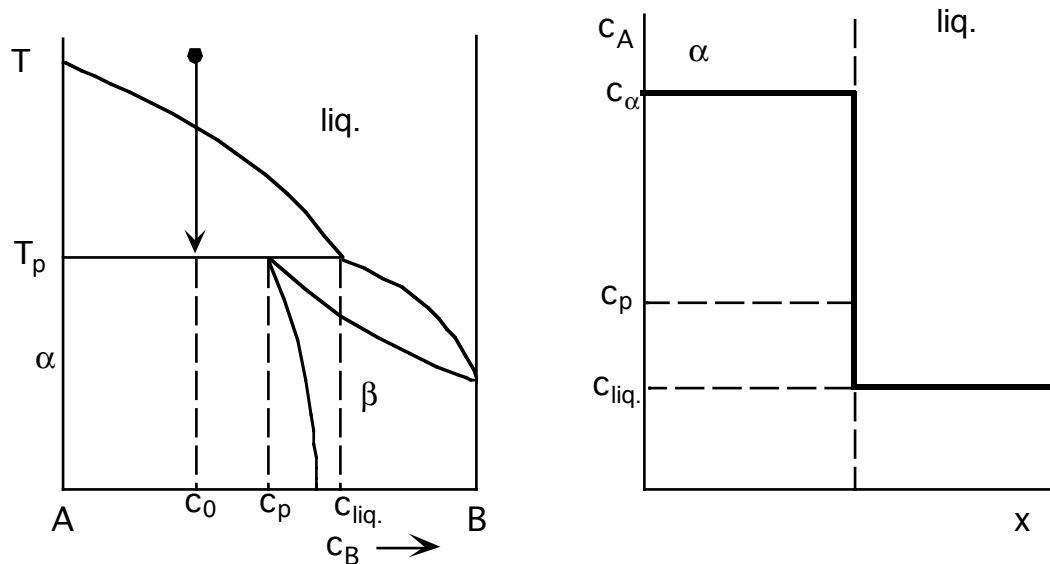
Consider two chemicals A and B that react with each other according to a second order reaction to form product AB. The process is designed to take place in a continuously stirred tank reactor (CSTR) with a capacity of 100 liters. The two reactants enter the CSTR in separate streams, each at a volume flow rate of 1 l/s. The concentration of A in the incoming stream is 15 mol/l and that of B is 25 mol/l, respectively. Calculate how many moles of A and B have been converted to product after flowing through the reactor. The reaction rate coefficient is  $0.02 \text{ s}^{-1}/\text{mol}$ .



**11.**

Consider the inter-diffusion of two species A and B. The chemical diffusion coefficient is adequately described by Darken's equation and the mixing behavior of the two components is described by the regular solution model, in which  $\ln \gamma_A = (\alpha/RT)x_B^2$ . The magnitude of the factor  $\alpha/RT$  is of the order of unity; it is positive in case the system tends to phase separate and it is negative in case it tends to form a compound. At the chosen temperature, the self-diffusion coefficients of A and B are  $10^{-8} \text{ cm}^2/\text{s}$  and  $2.5 \cdot 10^{-8} \text{ cm}^2/\text{s}$ , respectively. Determine whether diffusion of either species occurs faster in a mixture that tends to phase separate or that tends to form a compound, e.g., by comparatively evaluating the chemical diffusion coefficient at  $x_B = 0.5$ . Ignore correlation effects in self-diffusion.

12.



Consider a peritectic reaction  $\alpha + \text{liq.} = \beta$ , as illustrated in the above phase diagram. Assume that a melt of composition  $c_0$  is quenched to a temperature just above the peritectic temperature,  $T_p$ , and held there until the equilibrium is reached. The phases present are  $\alpha$  and liq., and their geometric arrangement is indicated in the adjacent schematic. Assume that the solid and liquid are perfectly separated, i.e., only one continuous and flat interface exists between them (simplest possible geometry). Now the temperature is dropped just below  $T_p$ . Obviously, phase  $\beta$  will now form.

- a) How will this happen. Illustrate the process by sketching composition vs. length diagrams at different times. (Hint: Ask yourself what phases will appear, which will disappear, which interface will move. Which components will diffuse into or out of which phases.)
- b) Assume some generic values for chemical diffusion coefficients in the liquid and solid of  $6.2 \cdot 10^{-5} \text{ cm}^2/\text{s}$  and  $2.5 \cdot 10^{-9} \text{ cm}^2/\text{s}$  respectively, and for the concentrations the values  $c_0 = 0.8$ ,  $c_p = 1.1$ , and  $c_{\text{liq.}} = 1.4 \text{ mol/cm}^3$ . Establish a simple but justifiable model that allows you to calculate the amount of phase  $\beta$  that forms as a function of time. Ignore the time required for nucleation.

13.

The crystal structure data for AlCu<sub>2</sub>Mn, a Heusler alloy, is listed below.

- What is the bravais lattice of this alloy?
- What will be the first five hkl that will appear in a diffraction pattern?
- What is the square modulus of the structure factor for each of the first five hkl?

<b>Spacegroup Symbol:</b>	F m $\bar{3}$ m
<b>Origin Offset:</b>	(none)
<b>Lattice Type:</b>	F

Unit Cell Parameters					
a [Å]	b [Å]	c [Å]	alpha [deg]	beta [deg]	gamma [deg]
5.9490	5.9490	5.9490	90.000	90.000	90.000

Fractional Coordinates of Atoms in the Asymmetric Unit				
Site Label	Element	x	y	z
Al	Al	0.0000	0.0000	0.0000
Cu	Cu	0.2500	0.2500	0.2500
Mn	Mn	0.5000	0.5000	0.5000

**14.**

Consider a cubic crystal structure with lattice parameter  $a=0.4$  nm. Xrays are generated using a Fe target ( $K\alpha$  radiation).

- a. Draw all reciprocal lattice points with indices up to 3 for the zone [001]. Make sure the points are drawn in the correct relative position.
- b. Draw to scale on the same drawing the radiation wave vector for an incident beam directed along the [100] direction. Also draw the corresponding Ewald sphere.
- c. What would be a possible direction for the incident beam so that the (130) reciprocal lattice point would fall on the Ewald sphere? (you may solve this by inspection or compute it)
- d. What is the diffraction angle for the reflection (130)

15.

Benzene,  $C_6H_6$ , is a molecular hydrocarbon and a liquid at standard atmospheric pressure and temperature. The lowest pressure allotrope of solid benzene crystallizes at 0.7 kbar at room temperature and has an orthorhombic  $Pbca$  ( $D_{152h}$ ) space group and four formula units per unit cell. Given x-ray diffraction determined literature values for the spacing between the (020), (200) and (111) planes of 0.478, 0.372 and 0.448 nm, respectively, determine the following:

- a. The values of the a, b and c lattice constants.
- b. The volume of the unit cell.
- c. The density of solid benzene.