Department of Materials Science and Engineering

DOCTORAL WRITTEN EXAM
January 23, 2014

Please follow these instructions:

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:

1. 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.

2. 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.

Name_____ **CODE NUMBER** _____

CHECK THE QUESTIONS YOU WISH TO HAVE GRADED:

Materials Physics And Chemistry:	Advanced Mechanical Behavior:
1. _____	4. _____
2. _____	5. _____
3. _____	6. _____

Advanced Thermodynamics Of Materials	Kinetics and Phase Transformations	Structure of Materials
7. _____	10._____	13._____
8. _____	11._____	14._____
9. _____	12._____	15._____

Materials Physics and Chemistry **Code_____**

1.

Density of states for 1D electron gas (i.e. a quantum wire): Consider a one-dimensional electron gas in which the electrons are restricted to move freely along the *z direction*. Derive the energy dependence of the density of states $g(E)$. [Hint: make a sketch first]

2.

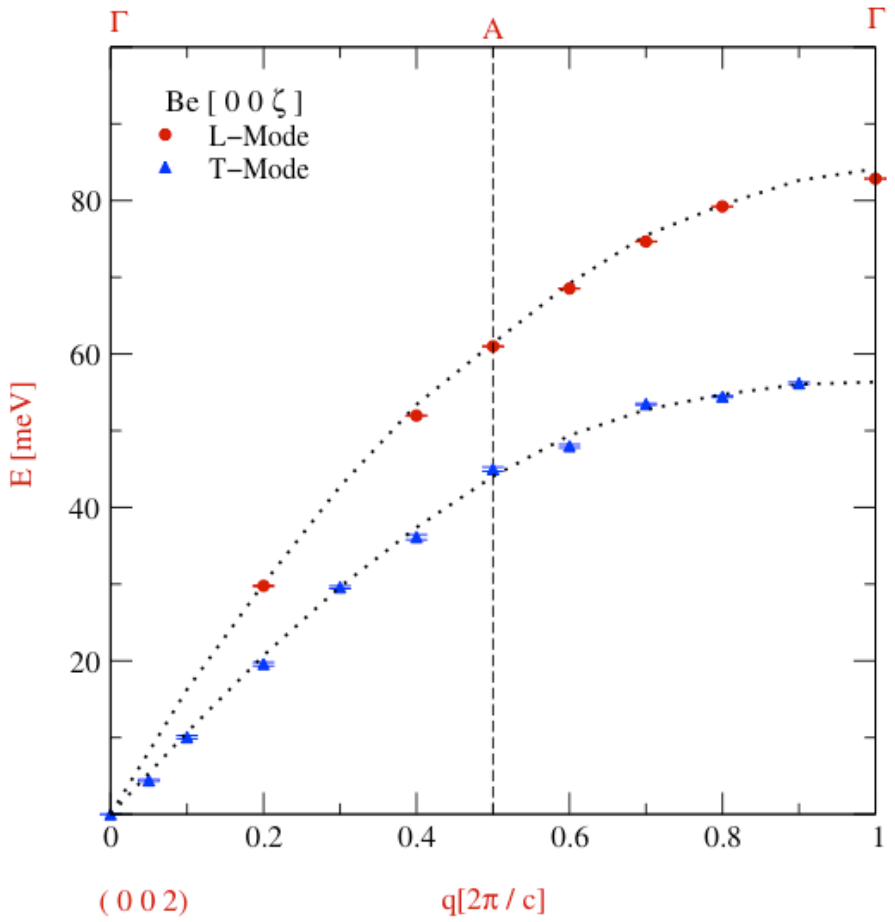
Band Structure The conduction and valence bands of a semiconductor are given by $E_c(k) = A + B\sqrt{1+(ak)^2}$ and $E_v(k) = -C\sqrt{1+(ak)^2}$, respectively, where $A = B = C = 1$ eV and $a = 1$ Å. The dielectric constant of the semiconductor is equal to 20. The electron scattering time is 10 fs.

a) Calculate the band gap of the semiconductor.
b) Is this a good light-emitting semiconductor? Explain. If yes, what is the wavelength of the emitted light?
c) Calculate the acceptor ionization energy.
d) If the conduction band has a concentration of 10^{19} cm^{-3} of free electrons, what is the electrical conductivity of this semiconductor?

Materials Physics and Chemistry **Code_____**

3.

The following curves show the room temperature phonon dispersion curves for a single crystal of beryllium in the [001] direction in both the longitudinal (L) and transverse (T) modes. The lattice parameter for beryllium in this direction is c=0.358 nm.



a) What phonon mode (T or L) is the fastest?

b) What are the velocities of these two modes in the low-frequency limit?

c) Describe an experiment or set of experiments that could be used to measure these phonon dispersion curves.

d) Suppose this crystal were heated up to just below the melting point. How would expect the shapes of these curves to change?

e) If the modulus of this sample was 50 GPa, and the density 4 gm/cm^3, what would be the expected velocity of sound?

f) If an acoustical phonon were propagating in the [001] direction, what would be its energy at the wavevector k_2?

g) What would be the energy of this same phonon at k=0?

h) What is the Debye temperature for this solid?

Advanced Mechanical Behavior **Code_____**

4. Answer all parts

a) Using a pure aluminum polycrystalline material as a baseline, calculate estimates of the individual increases in shear strength that arise from the various strengthening mechanisms that occur in an engineering aluminum alloy. The pure aluminum has a grain size of 100μm and a dislocation density of $10^{11}/m^2$. The engineered alloy has been processed to have a grain size of 10μm and a dislocation density of $10^{13}/m^2$. It has been heat treated to contain a maximum of 0.5 atomic percent of Mg in substitutional solid solution and 5 volume percent of non-deformable Mg_2Si precipitates with an average radius of 10nm. For the purposes of this problem, you may assume all strengthening mechanisms are independent.

The following may be helpful for your analysis
ky'=0.038MN/m3/2.
Young's Modulus = 70 GPa
Shear Modulus = 26.1 GPa
Poisson's ratio = 0.345
Burger's Vector = 0.286 nm
Solute hardening parameter of Mg atoms in Al = 0.5

b) What characteristics of the precipitate-matrix interface distinguish shearable vs non-deformable precipitates.

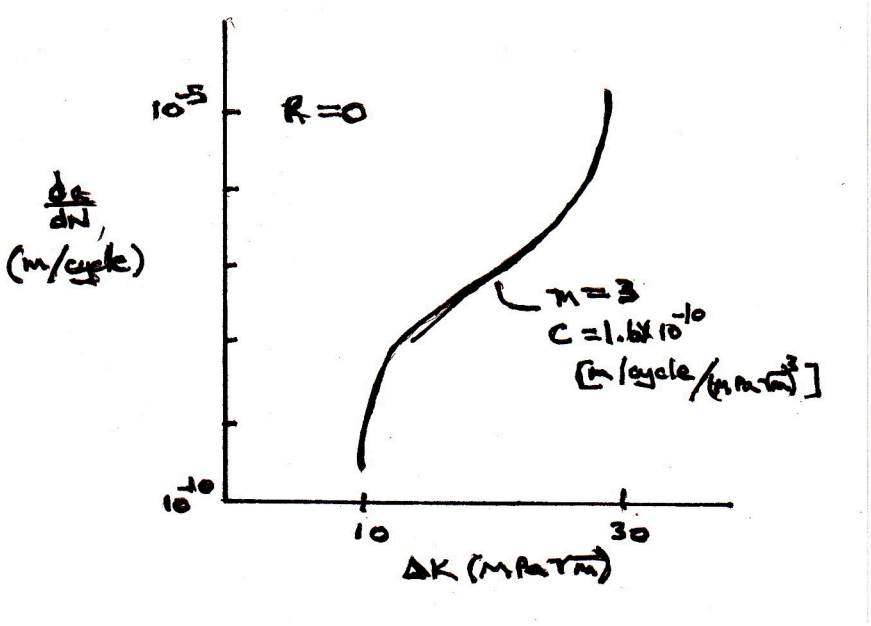
c) Sketch a complete age-hardening curve (shear strength vs aging time) for shearable and non-deformable precipitates and show (schematically) where these mechanisms operate.

Advanced Mechanical Behavior **Code_____**

5. Answer all parts

a) Assuming a cracked structure is subjected to a constant cyclic stress, $\Delta\sigma$, derive an analytical (closed form) expression for the number of cycles to propagate an initial crack, of length a_o, to final fracture at crack length, a_f. Please provide a rationale for all assumptions used.

b) You are estimating the feasibility of using a new aluminum alloy for an aircraft wing skin subjected to cyclic loading. Using the expression in part a) and information for this aluminum alloy provided in the figure provided below, estimate the number of cycles to propagate a crack, a_o, of length 0.02m to fracture when subjected to a cyclic stress range of 80 MPa at R=0. The K_{IC} of this material is 30MPa-√m.



c) A fracture toughness test was conducted on a titanium alloy that has a yield strength of 1000MPa. A center cracked panel was used for this test, with a half-crack length of 25mm. The panel width, W, was 50mm and the panel thickness was 15 mm. At this crack length the geometric correction factor, Y(a/W) was 1.2. The stress level at fracture was 200MPa. Calculate K_Q at fracture.

d) In part c, does this value qualify as a valid K_{IC} test? Explain your rationale.

Advanced Mechanical Behavior **Code_____**

6. Answer all parts

The critical resolved shear stress of aluminum is 1MPa.

a) An aluminum single crystal is subjected to a uniaxial tensile stress of σ_x = 250 kPa parallel to [100]. Calculate the value of σ_x at which slip will initiate in this single crystal.

b) Estimate the yield strength of pure aluminum in a polycrystalline form (grain size effects should be considered negligible). Provide a rationale for this estimate.

c) Is the following dislocation reaction likely to occur? Show why or why not.

$$\frac{a}{2}[\bar{1}01] \rightarrow \frac{a}{6}[\bar{2}11] + \frac{a}{6}[\bar{1}\bar{1}2]$$

d) A stacking fault is created when one dislocation line splits into partial dislocations with two separate Burgers vectors. Will a material with a high stacking fault energy have partials with large spacing or small spacing? Explain your rationale.

e) Describe the impact of the stacking fault energy on work hardening of metals.

7.

The calcination of $CaCO_3$ occurs spontaneously at 1150K according to the reaction

$CaCO_3 = CaO + CO_2$ $\Delta H_{calc.}(298) = 178{,}100$ J/mol

To heat $CaCO_3$ to the decomposition temperature we use coal, which releases heat upon combustion according to

$C + O_2 = CO_2$ $\Delta H_C(298) = -393{,}500$ J/mol

$CaCO_3$, O_2, and C enter the process at room temperature. Calculate the amount of coal needed to run this process. Assume that the temperature of the reaction products does not exceed 1150 K. Of the heat capacities below, some or all may be needed to solve the problem.

$c_{p(CaO)} = 49.6 + 0.0045T$ $c_{p(O_2)} = 29.96 + 0.0041T$

$c_{p(CO_2)} = 44.14 + 0.009T$ $c_{p(CaCO_3)} = 112.4 + 0.021T$

$c_{p(Ca)} = 25.4 + 0.0073T$ $c_{p(C)} = 24.43 + 0.0004T$.

8.

Bi and Cd form a binary eutectic with essentially no mutual solubility in the solid state. The eutectic temperature is 406 K and the melting temperature of Bi is 560 K. The melting enthalpy is 10,900 J/mol. The heat capacities at constant pressure of liquid and solid Bi are 20 and 18 J/molK respectively. Calculate the composition of the eutectic liquid mixture (i.e., the liquidus for Bi at 406 K).

9.

Consider a two-component system, consisting of two *A*-type and two *B*-type particles. *A*-type particles can assume energy levels $\varepsilon_{1A} = 0$, $\varepsilon_{2A} = \varepsilon$, $\varepsilon_{3A} = 2\varepsilon$, $\varepsilon_{4A} = 3\varepsilon$, and $\varepsilon_{5A} = 4\varepsilon$, and $\varepsilon_{1B} = 0$, $\varepsilon_{2B} = 2\varepsilon$, $\varepsilon_{3B} = 4\varepsilon$,. Among their own species, both *A* and *B* particles are indistinguishable. Assume in terms of magnitude, $\varepsilon = k_B T$.

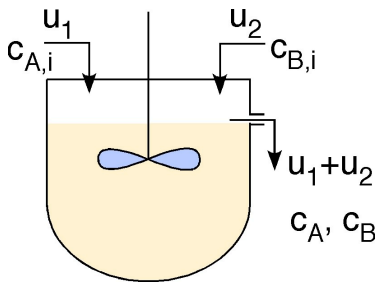
a) calculate the partition function of the combined *AB* system. All energy levels listed above can be occupied according to species identity.

b) Calculate the average energy of the *AB* system in units of ε.

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 s^{-1}l/mol.



Kinetics and Phase Transformations **Code _____**

11.

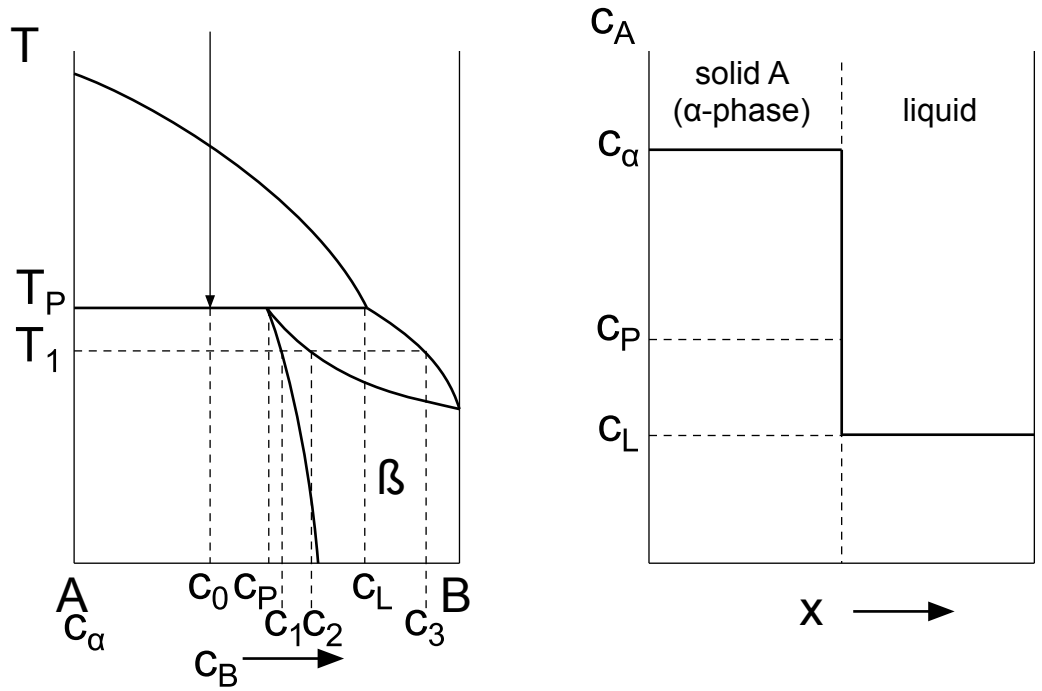
The oxidation of Zn to form ZnO occurs via interstitial diffusion of Zn in ZnO towards the oxide/gas interface. The defect equilibrium is described by

$$Zn_i^{\bullet} + e^- + \frac{1}{2}O_2 \longleftrightarrow ZnO \qquad \text{with } \Delta G^\circ = -380900 + 34.8T \text{ (J/mol)}$$

At 800K the fraction of occupied interstitial sites in ZnO at the metal/oxide interface is $2 \cdot 10^{-5}$. ZnO has a density of 5.58 g/cc at this temperature. Assuming an average distance between interstitial sites of 2.8 Å, a Debye temperature of the compound of $\theta_D = 416$ K, and an activation energy of migration for interstitial Zn of 400 kJ/mol, calculate the time it takes for the oxide layer on Zn to reach a thickness of 1 μm.

Kinetics and Phase Transformations **Code_____**

12.



Consider a peritectic reaction α + liq. = β, as illustrated in the above phase diagram (α-phase is pure A). 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 α 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, say T_1. Obviously, phase β will now form.

a) How will this happen. Illustrate the process by sketching composition vs. length diagrams at different times. (Hint: examine what phases will appear or disappear, and which way the 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 $6.2 \cdot 10^{-5}$ cm^2/s and $2.5 \cdot 10^{-9}$ cm^2/s respectively, and for the concentrations the values $c_0 = 0.8$, $c_p = 1.1$, $c_1 = 1.14$, $c_2 = 1.2$, $c_{L.} = 1.4$, and $c_3 = 1.6$ mol/cm^3. Establish a simple but justifiable model that allows you to calculate the amount of phase β that forms as a function of time. Ignore the time required for nucleation.