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, January 26, 2012

Department of Materials Science and Engineering

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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 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.______

Materials Physics and Chemistry **Code_______**

1.

a) Name a semiconductor that can be used for the emission of each of the following types of electromagnetic radiation: infrared, red, blue, ultraviolet.
b) Draw the optical absorption spectrum of Si and GaAs.
c) Draw the band diagram for a silicon solar cell under bright and dark conditions. Describe how light is converted to electricity.
d) How would you measure if a semiconductor is n-type or p-type?
e) A bulk semiconductor has a 1 eV band gap. The conduction-band effective mass is 0.1 m_e and the valence band effective mass is 0.5 m_e. Calculate the band gap for the following nanostructures made with this semiconductor:
    a. a slab with thickness of 5 nm
    b. a nanowire with a square cross section of 5 nm sides
    c. a cubic quantum dot with 5 nm edges

2.

a) Derive the Drude equation for electrical resistivity. Estimate the value of the conductivity of Cu at room temperature.
b) Do you expect diamond to have a higher electrical conductivity than silicon at room temperature? Why or why not?
c) Draw the dependence of the electron scattering time on temperature and explain the main source of scattering in each temperature regime.
d) Draw the specific heat of aluminum as a function of temperature. Give the functional dependence for each regime.
e) How would you measure the phonon frequencies of a material as a function of wave vector?

3.

a) Imagine a chain of carbon atoms, where the nearest-neighbor atoms are separated by a distance of 0.154 nanometers (you can assume that it's a linear chain), and connected by linear springs having a constant k_{spr}. Derive and graph a 1-dimensional phonon dispersion diagram for this system.

b) Do the same thing as in Part (a), but this time imagine that silicon atoms replace carbon atoms.

c) Do the same thing as in Part (a), but this time imagine that the chain is –C–Si–C–Si–... That is, an alternating sequence of carbon and silicon atoms.

d) Which of the systems above have a higher thermal conductivity? Why?

e) Rank these in order of their thermal conductivities, and explain your answer: Diamond, Silicon, Polyethelene, Silicon Carbide.

4.

Assume that the uniaxial true stress-true strain tensile response is given by

$$\sigma_T = K\,\varepsilon_T^{\,n}$$

a) Derive an expression for the true stress at necking in terms of the materials tensile strength (in engineering stress) and strain hardening exponent.

b) Show that the true strain at necking, ε_T , equals the strain hardening exponent, n.

c) From this result describe the interrelationship between the tendency of a material to neck and its work hardening characteristics.

5.

A gas turbine aircraft engine has a metallic component subjected to a sustained stress of 100MPa at a temperature of 600°C that induces a steady state creep strain rate of $3x10^{-8}$/sec. The material has been processed to provide a grain size of 10μm. The creep mechanism at this temperature is Coble creep with an activation energy of 75kJ/mole.

a) If the stress is increased to 150MPa and the temperature to 700°C calculate the expected creep rate?

b) At a stress of 100MPa and temperature of 600°C, the designer requires a steady state creep strain rate of $1x10^{-9}$/sec. It has been proposed that the component be processed to change the grain size to achieve this steady state creep rate. Determine if this would be an effective strategy and, if so, what grain size would be required. Show calculations to support your conclusion.

6.

a) Provide a sketch of a dislocation loop in the form of a circle and specify the Burgers vector of the loop. Denote the portions of the loop that are edge and those that are screw in nature. Provide relationships for the energy of the screw and edge dislocations. Based on these energies would you expect dislocation loops to be generally circular in shape. If yes, explain your reasoning. If no, show how the loop you have drawn will change its shape because of energy differences along the circumference.

b. Consider dislocations advancing by the lateral spreading of kinks. Let the advanced portion of the dislocation line be a distance d beyond the portion of the line that has not advanced and let the kinks be separated by a distance L along the line (i.e. the kink density per unit length is L^{-1}). Draw a schematic of this situation. Determine a relationship between the dislocation velocity, v_d, and the kink velocity v_k.

7.

A paramagnet in an environment at constant T and P is placed in a magnetic field with strength H_1. After the paramagnet has equilibrated with the environment in the magnetic field H_1, the magnetic field is suddenly switched off.

How much heat is exchanged between the paramagnet and the environment between the time that the magnetic field is switched off and the paramagnet reaches a new equilibrium state with the environment at zero magnetic field.

You can assume that the following response functions of the paramagnet are constants in the temperature, pressure and magnetic field intervals of interest:

$$\chi = \frac{1}{V_o}\left(\frac{\partial \mathrm{M}}{\partial \mathrm{H}}\right)_{T,P}, \qquad \gamma = \frac{1}{V_o}\left(\frac{\partial \mathrm{M}}{\partial T}\right)_{P,\mathrm{H}}, \qquad \delta = \frac{1}{V_o}\left(\frac{\partial \mathrm{M}}{\partial P}\right)_{T,\mathrm{H}}, \qquad \kappa = -\frac{1}{V_o}\left(\frac{\partial V}{\partial P}\right)_{T,\mathrm{H}},$$

$$\beta = \frac{1}{V_o}\left(\frac{\partial V}{\partial T}\right)_{T,\mathrm{H}}, \qquad c_{P,\mathrm{H}} = \frac{T}{V_o}\left(\frac{\partial S}{\partial T}\right)_{P,\mathrm{H}}$$

V_o is the volume of the paramagnet at T, P but at zero magnetic field.

8.

Derive an expression for $\left(\frac{\partial T}{\partial P}\right)_U$ in terms of measurable response coefficients (e.g. C_p, β, κ etc.) and easily measurable thermodynamic state variables. (*T* is the temperature, *P* is the pressure and *U* is the internal energy).

9.

A linear polymer is made up of M monomers. The electrons of the covalent bonds in each monomer can be in one of two states: a ground state with energy ε_o and an excited state with energy ε_1. The equilibrium length of each monomer is l_o in the ground state and l_1 in the excited state. The covalent bond within each monomer has a force constant f_o in the ground state and f_1 in the excited state (that is when the spacing between the atoms within each monomer deviates from its equilibrium value by ξ, the energy of the bond increases harmonically by $\frac{1}{2} f \cdot \xi^2$). The effective mass of the vibrating bonds is m.

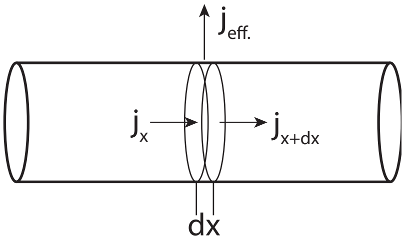
a) Assume that all monomers stay in their electronic ground state (i.e. $\varepsilon_1 >> \varepsilon_o$ such that the electrons of the monomers are never excited out of their ground state). Derive a closed form expression for the partition function of the linear polymer at constant temperature T and fixed polymer length M. You can assume that the ends of the polymer are at constant force F=0.

b) Now assume that the electrons of the monomers can be excited. At constant temperature T and fixed polymer length M, rederive an expression for the appropriate partition function. Again you may assume that the ends of the polymer are at constant force F=0. Make sure to derive a closed form expression by summing over all microstates.

c) Write down an expression for the probability $\mathrm{P}(N)$ that N monomers are in their excited electronic state.

10.

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 m^3/s.



a) 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.

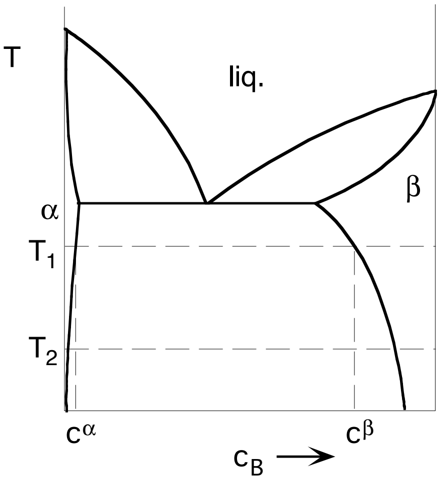
b) Calculate the length of the tube needed to reduce the N_2 concentration to 1/32 of its initial value. The molecular weight of N_2 = 28 g/mol.

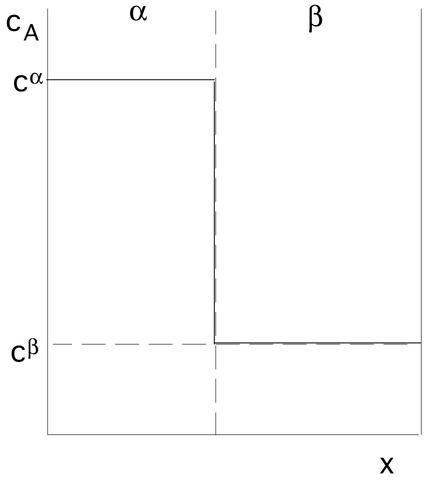
11.

Consider the geometric configuration of two phases α and β given in the diagram below (right hand side). This configuration corresponds to a situation in equilibrium at T_1 of the adjacent phase diagram. The system is cooled abruptly to T_2.

a) Superimpose the concentration profile after some time (sufficient for the effects to be visible, but still far from equilibrium). Make sure the direction of migration of the interface is obvious from your sketch.

b) Develop an expression for the velocity of migration of the interface based on the diffusivity of A in β. Assume that the change in solubility of B in α is negligible.





12.

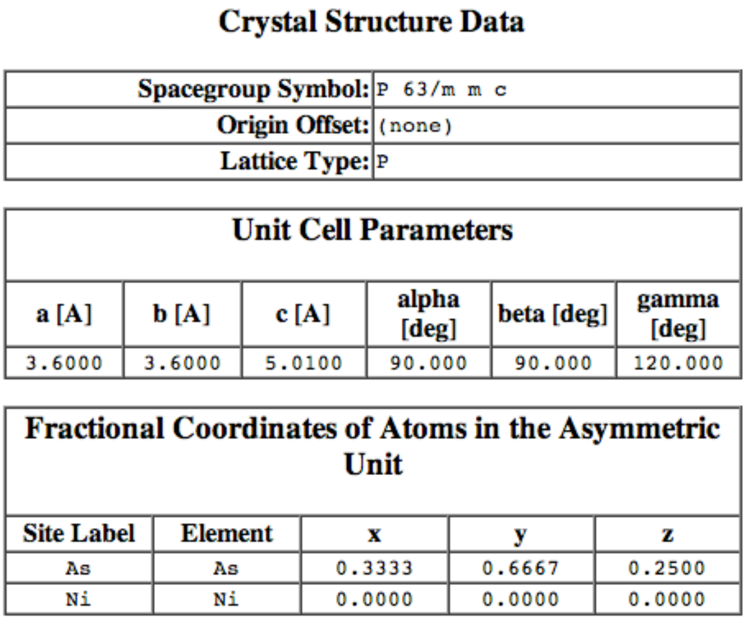
Consider a nickel sheet of a thickness 4 mm. It contains 6 at.% of silicon dissolved on interstitial positions. The sheet is sandwiched between two infinitely thick slabs of nickel and heated to 1000°C. The diffusion coefficient of Si in Ni is $6.8 \cdot 10^{-9}$ cm^2/s. Calculate the total amount of Si that has diffused out of the central sheet after 12 hours.

(Hint: the following relationship $\int \operatorname{erf} z \, dz \equiv \int 1 \cdot \operatorname{erf} z \, dz$ may be useful, in that it allows for integration by parts of erf$z$.

13.

The crystal structure data for NiAs, is listed below.

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



Crystal Structure Data

Spacegroup Symbol:	P 63/m m c
Origin Offset:	(none)
Lattice Type:	P

Unit Cell Parameters

a [A]	b [A]	c [A]	alpha [deg]	beta [deg]	gamma [deg]
3.6000	3.6000	5.0100	90.000	90.000	120.000

Fractional Coordinates of Atoms in the Asymmetric Unit

Site Label	Element	x	y	z
As	As	0.3333	0.6667	0.2500
Ni	Ni	0.0000	0.0000	0.0000

14.

Consider a hexagonal crystal structure with lattice parameter a=0.4 nm and c=0.6nm. Xrays are generated using a Fe target (Kα 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 (210) 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

15.

For the Lanthanum Cuprate please find the following:

a. to determine the spacing between the (110) planes
b. show the symmetry elements in the unit cell with respect to the lattice vectors, and the atomic positions in the projection along the c-axis
c. Determine the lattice parameters and the Bravais lattice for the primitive unit cell for this structure

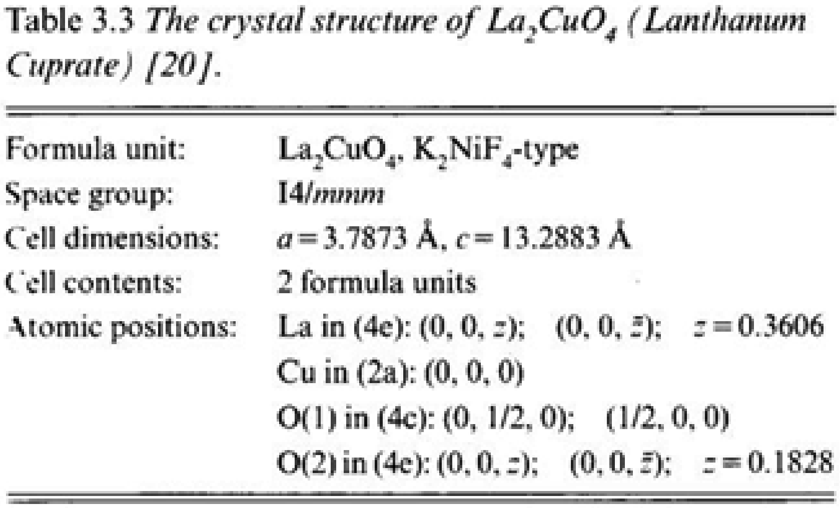


Table 3.3 *The crystal structure of La_2CuO_4 (Lanthanum Cuprate) [20].*

Formula unit:	La_2CuO_4, K_2NiF_4-type
Space group:	I4/*mmm*
Cell dimensions:	$a = 3.7873$ Å, $c = 13.2883$ Å
Cell contents:	2 formula units
Atomic positions:	La in (4e): $(0, 0, z)$; $(0, 0, \bar{z})$; $z = 0.3606$
	Cu in (2a): $(0, 0, 0)$
	O(1) in (4c): $(0, 1/2, 0)$; $(1/2, 0, 0)$
	O(2) in (4e): $(0, 0, z)$; $(0, 0, \bar{z})$; $z = 0.1828$