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 24, 2012

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. ______

Materials Physics and Chemistry **Code_______**

1.

Estimate the proportion of valence electrons that participate in 3D electrical conduction in Na metal at 300K, using Fermi- Dirac statistics, and the following parameters:

Fermi Energy = 3.22 eV
Electron concentration = 2.65 x 1022 /cm^3

a) Determine the energy which corresponds to an occupation probability of f=0.9
b) Determine the number of electrons with energies greater than the value determined in (a). Note that you may approximate the FD distribution function, f(E)~f from (a).
c) Calculate the proportion of valence electrons that participate in electrical conduction.
d) How do your results in (a)-(c) change if the dimensionality of conduction is restricted to 2D? Show your work.

2.

An incandescent light bulb works by heating a tungsten wire to 3000K until it glows white-hot. Assume that the wire is an ideal blackbody. The length of the (uncoiled) wire is 500 mm and its diameter is 0.05 mm

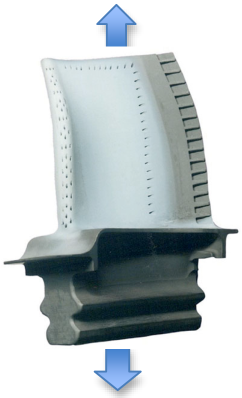
a) What is the wavelength of the peak of the spectral distribution?
b) What is the total emitter power of the light bulb?
c) What fraction of the emitted radiation is visible to humans (i.e. what is the efficiency of the light bulb)?
d) What would be the total emitted power and peak wavelength if the temperature could be increased to 4000 K? Can the temperature be increased to 4000 K and if not why?

3.

a) Graph the reflectivity spectrum (i.e. intensity versus wavelength in nanometers) of a thin film of a generic alkali metal. Use Drude theory to explain its main features. (Show all work)
b) For the material in Part (a), graph the total absorbed light intensity versus thickness of the film.
c) Using the same x-axis as in Part (a), graph the absorption spectrum of GaAs (Eg = 1.43 eV). Explain its main features.
d) Graph the absorption spectrum of n-type doped GaAs. Assume the dopant atoms are fully ionized.

4.

Question 1: A nickel-based superalloy aircraft engine turbine blade is manufactured using a casting process that produces an aligned single crystal. The stresses are sufficiently low that the blades are elastically loaded. The preferred orientation along the blade loading axis is one in which the Young's modulus is minimized. This is required to minimize thermal stresses developed during engine-start up and shut down.



Loading Axis

Assume:

$C11 = 246.5$ GPa
$C12 = 147.3$ GPa
$C44 = 124.7$ GPa
$S11 = 0.0073\ \text{GPa}^{-1}$
$S12 = -0.0027\ \text{GPa}^{-1}$
$S44 = 0.0080\ \text{GPa}^{-1}$

a) Using the information provided and your knowledge of elastic anisotropy in single crystals - what crystallographic alignment would you recommend? Support your recommendation with a calculation or calculations.

b) Calculate the elastic modulus in this direction?

c) If this stress in the loading axis is assumed to be uniaxial and equal to 100 MPa, calculate the strain in the loading direction.

5.

You are a member of a team developing computational tools for simulating the extrusion of magnesium components at room temperature. During extrusion magnesium is subjected to high strains under a complex stress state that inhibits fracture in this normally fracture-prone material. Your assignment is to recommend a simple testing approach (not an extrusion) for experimentally measuring the plastic flow characteristics of this material at high strains, while inhibiting fracture. Recommend a test method and explain your rationale in terms of the maximum shear stress and mean pressure. Include a description of the stress state in your test and a Mohr's circle representation.

6.

<u>Note: complete all parts (a through d!</u>):

The following tensile yielding loads were determined for various orientations of pure aluminum single crystals. The single crystals were in the form of cylinders, 20mm in diameter.

ϕ	λ	Load (N)
83.5	18	2969
70.5	29	1107
60	30.5	746
50	40	655
29	62.5	777
5	85.5	4079

a) From this data determine the critical resolved shear strength of single crystal aluminum.

b) From the above, calculate the yield strength of pure aluminum in a polycrystalline form.

Question 3 continues on next page

Question 3 continued:
c) Two aluminum single crystals are pulled in tension. The tensile axis in one crystal is oriented in a <123> direction, the other is in a <111> direction. Locate (approximately) these crystal orientations on a standard stereographic triangle.

d) Draw a schematic of the shear stress vs. shear strain behavior of these two single crystal samples and describe their response in terms of the first two stages of single crystal slip.

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:

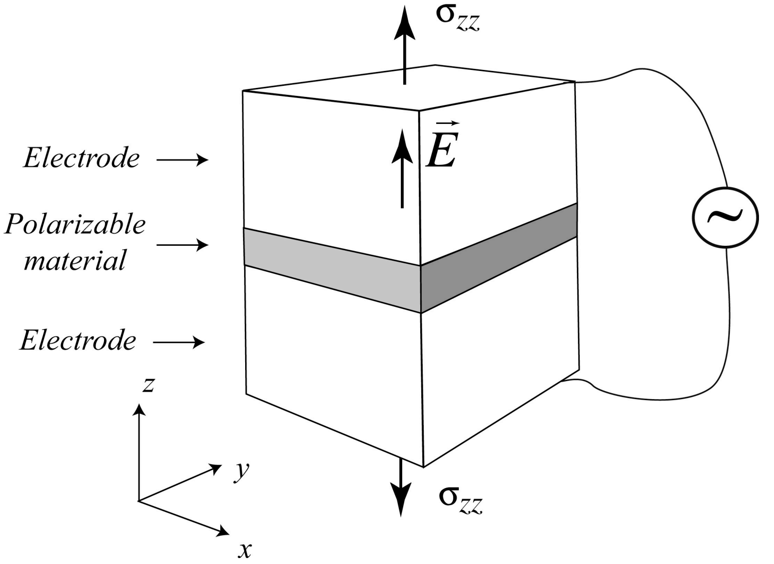
$$\chi = \frac{1}{V_o}\left(\frac{\partial \mathrm{M}}{\partial \mathrm{H}}\right)_{T,P}, \qquad \gamma = \frac{1}{V_o}\left(\frac{\partial \mathrm{M}}{\partial T}\right)_{P,\mathrm{H}}, \qquad \delta = \frac{1}{V_o}\left(\frac{\partial \mathrm{M}}{\partial P}\right)_{T,\mathrm{H}}, \qquad \kappa = -\frac{1}{V_o}\left(\frac{\partial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

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

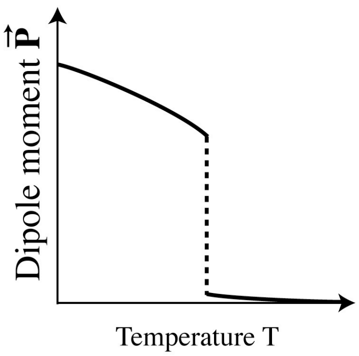
V_o is the volume of the paramagnet at T, P but at zero magnetic field.

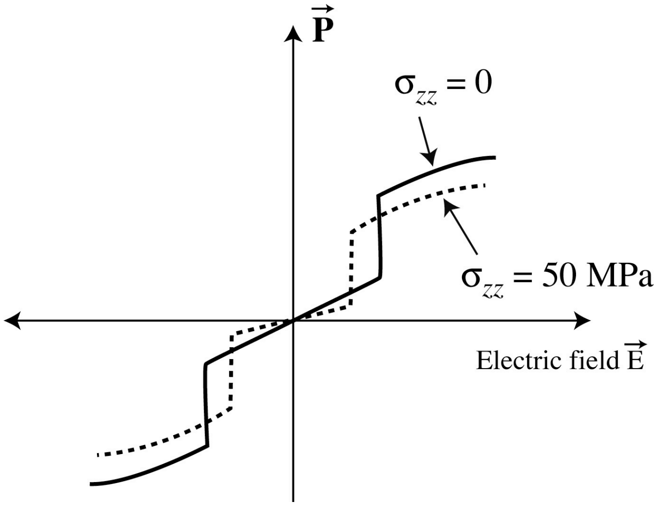
8.

An electrically polarizable material (electronic insulator) that undergoes a ferroelectric (α-phase) to paraelectric (β-phase) phase transition is coherently wedged between two large electrodes. The interfaces between the polarizable material and the two electrodes are coherent (i.e. perfect atomic matching across the interface).



The plots below show the variation of the dipole moment of the polarizable material as a function of temperature (at zero electric field) and as a function of electric field (at constant temperature). It is possible to impose a stress on the polarizable material along the z-axis. The dashed line in the P versus E plot is measured at a tensile stress of 50 MPa while the solid line is measured at zero stress.





(A ferroelectric material has a finite dipole moment even when the electric field is zero, while a paraelectric material only has a dipole moment in an electric field and for small electric fields its dipole moment is proportional to the electric field).

a) Which phase has a larger thickness along the z-axis (explain your answer)?
b) Schematically plot a temperature versus electric field phase diagram.

9.

A block of fcc iron is placed in a nitrogen rich gas with a constant nitrogen chemical potential μ_N. Nitrogen atoms can fill octahedral interstitial sites in the fcc crystal of Fe. Assume there are M Fe atoms such that there are M octahedral interstitial sites. The energy of M iron atoms in the fcc crystal is E_o. Addition of each nitrogen atom to the fcc crystal leads to an increase in energy by ε. The concentration of nitrogen atoms that fill octahedral sites in the Fe crystal is very dilute so that interactions among different nitrogen atoms can be neglected. Denote the number of interstitial nitrogen atoms at any moment in time by N. Assume the crystal is at constant temperature T and fixed volume V.

a) Derive an expression of the appropriate partition function for the block of iron with interstitial nitrogen (actually get a closed form analytical expression) under the imposed thermodynamic boundary conditions described above.

b) Use the expression for the partition function from part (a) to determine the equilibrium number of interstitial nitrogen atoms as a function of nitrogen chemical potential μ_N and temperature T (if you were unsuccessful in part (a), then write out formally how you would derive such an expression).

10.

Hydrogen gas molecules impinge upon the surface of a stabilized zirconia membrane containing 15 mol-% CaO, where they react with oxygen according to $H_2 + O_O^{'''} \rightleftarrows H_2O + V_O + 2e^-$, as long as the velocity component normal to the surface provides a kinetic energy in excess of 150 kJ/mol.

a) Use the collision rate theory to calculate the value for the reaction rate coefficient *k* as defined in the following rate equation $\frac{1}{A}\frac{dn_O}{dt} = -k\theta_{O^{2-}}c_{H_2}$, where c_{H_2} is the concentration of hydrogen in the gas phase and $\theta_{O^{2-}}$ is the fraction of oxygen at the surface of zirconia occupying stable (extrinsic) oxygen vacancies. Assume a temperature of 1200 K.

b) Given a linear gas flow velocity of 0.01 m/s, an inner tube radius of 0.01 m, and a pressure of 1 10^5 Pa, calculate the length of the tube by which the hydrogen concentration has decreased to half its inlet value (e.g., 100% pure H_2). Assume that hydrogen behaves like an ideal gas.

11.

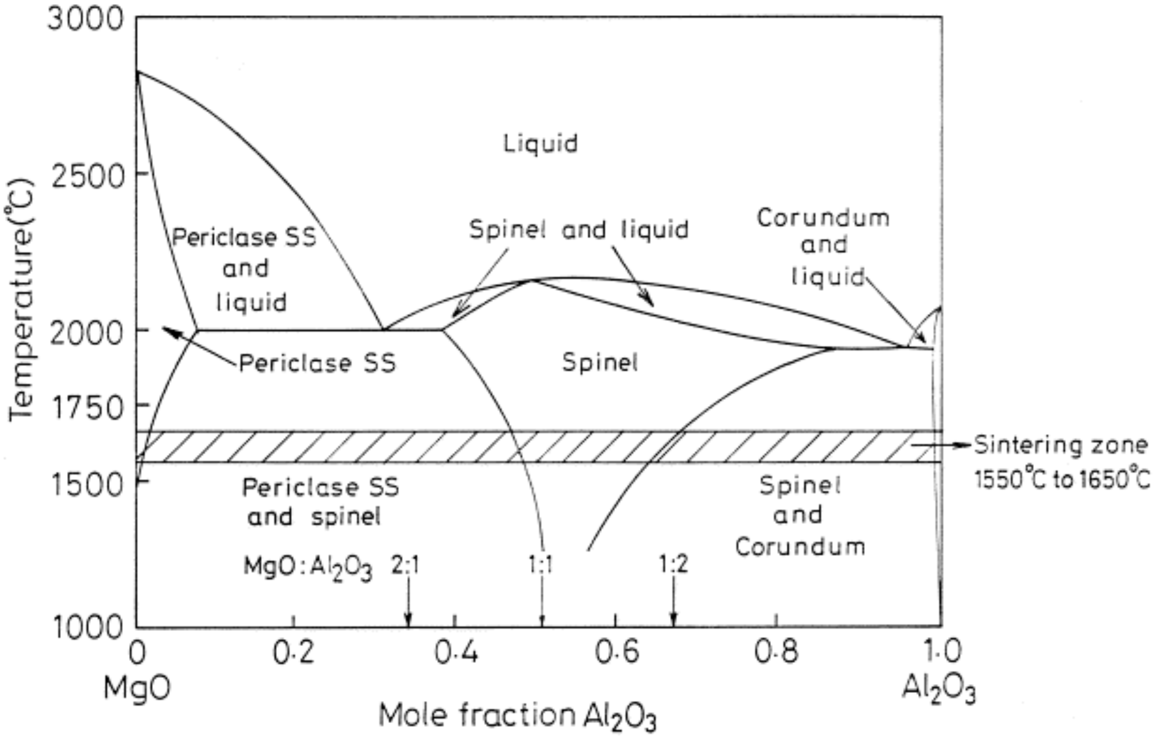
Magnesium oxide (MgO) and aluminum oxide (Al_2O_3) form spinel ($MgAl_2O_4$) via solid-state reaction:

$$MgO + Al_2O_3 \xrightarrow{k} MgAl_2O_4$$

a) Assuming that the rate-limiting mechanism in spinel growth consists of the diffusion of Al and Mg cations across the spinel layer in opposite directions, while maintaining charge neutrality, devise a simple kinetic rate equation that yields the thickness of the spinel layer as a function of time. Assume planar interfaces and one-dimensional fluxes.

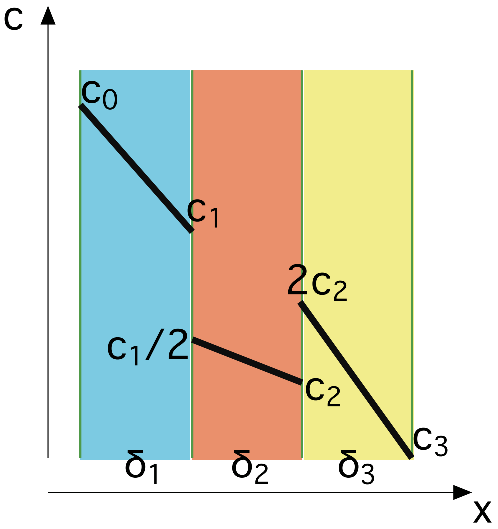
b) Given the densities of MgO, Al_2O_3, and $MgAl_2O_4$ as 3.58 g/cc, 3.95 g/cc, and 3.6 g/cc, respectively (you may not need all these densities to solve the problem), and assuming effective diffusion coefficients of 10^{-9} cm2/s and $6 \cdot 10^{-9}$ cm^2/s for Al and Mg, respectively, at 1600°C, calculate the time it takes for the spinel layer to reach a thickness of 50 μm.

The MgO-Al_2O_3 phase diagram is given below. For simplicity assume that the in spinel compositions that are at equilibrium with MgO and Al_2O_3 are described by MgO:Al_2O_3 ratios of 1:1 and 1:2, respectively. Also given, the atomic weights of Mg, Al, and O are 24, 27, and 16 g/mol, respectively.



12.

Consider the diffusion of Li^+ ions through a composite membrane. The membrane consists of three layers characterized by diffusion coefficients $D_1 = 2 \cdot 10^{-4}$ cm^2/s, $D_2 = 5 \cdot 10^{-4}$ cm^2/s, and $D_3 = 10^{-4}$ cm^2/s, and thicknesses $\delta_1 = 0.1$ cm, $\delta_2 = 0.2$ cm, and $\delta_3 = 0.15$ cm. Furthermore, the solubility of Li^+ in the central layer (2) is half that of the two other layers (1 and 2). Thus a concentration of c_1 in layer 1 is in equilibrium with a concentration $c_1/2$ in layer 2 at the interface between 1 and 2, and similarly, a concentration c_2 in layer 2 is in equilibrium with $2 \cdot c_2$ in layer 3 at the interface between 2 and 3.



a) Derive the expression that describes the stead-state molar flux j_{Li} across the composite wall as a function of the concentration difference between c_3 and c_0.

b) Assuming that c_0 is 1 mol/cm^3 and $c_3 = 0$ mol/cm^3, calculate the magnitude of the steady-state Li^+ flux across this membrane.

13. No test takers

14.

15.