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 30, 2009

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. **<u>You must submit 2 questions from each core area you are taking for grading</u>**. You will have 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 <u>all</u> 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 <u>all</u> other exam pages in the other side of your folder, and return <u>everything</u> to Renee if you finish before your time is up.

<u>Please be sure to complete the information required on each page</u>.

CODE NUMBER ________________

<u>CHECK THE QUESTIONS YOU WISH TO HAVE GRADED:</u>

Materials Physics <u>And Chemistry:</u>

1. _____
2. _____
3. _____

Advanced Mechanical <u>Behavior:</u>

4. _____
5. _____
6. _____

Advanced Thermodynamics <u>Of Materials</u>

7. _____
8. _____
9. _____

Kinetics and Phase <u>Transformations</u>

10. ______
11. ______
12. ______

<u>Structure of Materials</u>

13. ______
14. ______
15. ______

Materials Physics and Chemistry **Code________**

1.

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.

2.

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 (E_g = 1.43 eV). Explain its main features.

3.

Light strikes a clean surface of a semiconductor. An electron detector (for example, a simple metal plate) is positioned above the surface, and the apparatus is in vacuum. Draw a diagram of the set-up and answer the following questions; show all work:

a) Graph the electrical current in the detector versus wavelength (in nanometers) of the incident light. Label all important features of the curve and explain their significance.

b) Graph the velocity of the electrons striking the detector versus incident wavelength. Label all important features of the curve and explain their significance.

c) If the semiconductor is GaAs (E_g = 1.43 eV) doped with phosphorus, repeat parts (a) and (b) versus the concentration of phosphorus atoms. (Assume complete ionization.)

4.

a) Is the following dislocation reaction possible? Show why or why not.

$$\frac{a}{2}[11\bar{1}] + \frac{a}{2}[11\bar{1}] \rightarrow a[100]$$

b) If one dislocation line splits into partial dislocations with two separate Burgers vectors, a stacking fault is created. Will a material with high stacking fault energy have partials with large spacing or small spacing?

5.

a) Assume that a bcc crystal slips on {110} <111>. For a tensile axis parallel to the {123} crystal axis, calculate the Schmid factor for all possible slip systems. (Hint: Use of a stereographic projection is recommended.)

b) Is this crystal oriented for single slip or for multiple slip?

c) What is the conjugate slip system for tensile deformation if the initial tensile axis is parallel to the {123} crystal axis?

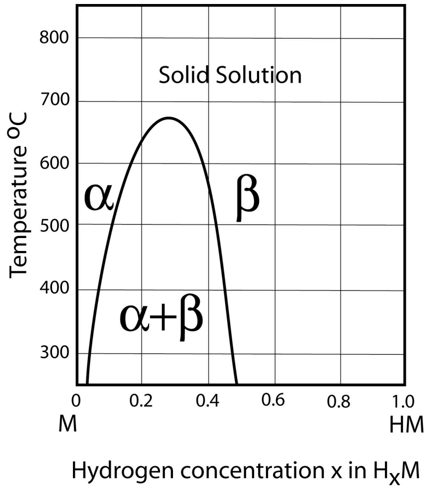
d) What is the conjugate slip system for compressive deformation if the initial compression axis is parallel to the {123} crystal axis?

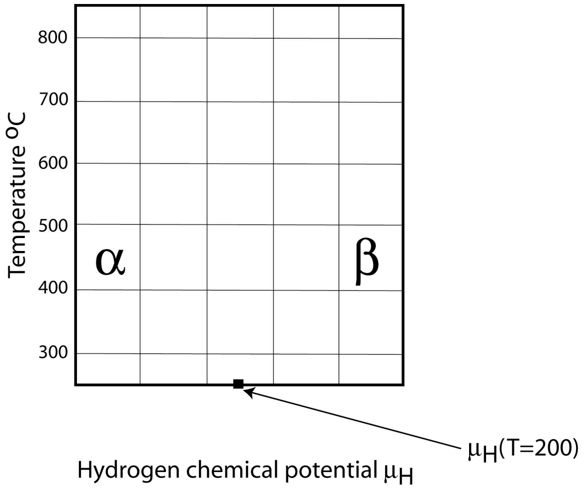
6.

An engineering component made of an alloy steel is subject to creep under simple tension at a stress of 150 MPa. What is the highest temperature that can be permitted if the component must function for 40 days, and a safety factor of 10 on its life is required? The same material was subjected to creep in a test at 150 MPa at 530°C, in which is ruptured in 260 hours.

7.

Hydrogen can fill the interstitial sites of many metals. The figure below on the left illustrates a typical metal-hydride phase diagram (at constant pressure), in this case exhibiting a miscibility gap between a metal with a dilute hydrogen concentration (α) and the same metal with a significantly higher hydrogen concentration (β). x is the fraction of interstitial sites of the metal M occupied by hydrogen. Above 675 C a complete solid solution forms.





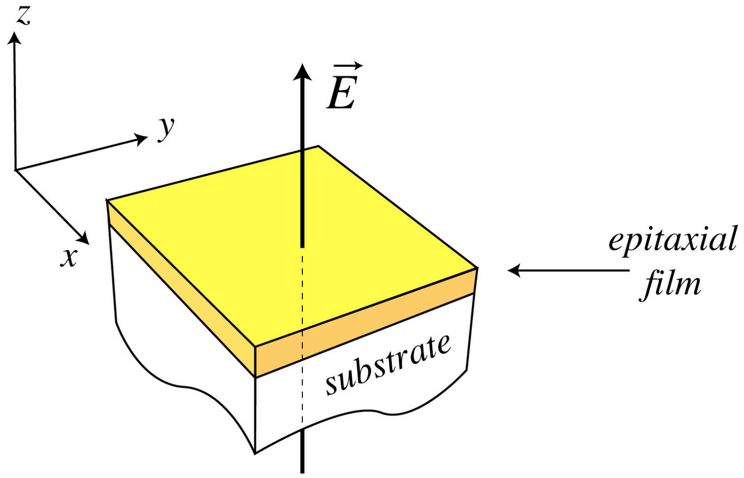
Convert the T versus x phase diagram on the left (temperature versus hydrogen composition) into a T versus μ_H phase diagram (temperature versus hydrogen chemical potential). In a T versus μ_H phase diagram, α is stable at low hydrogen chemical potential while β is stable at high hydrogen chemical potential. The filled square in the phase diagram on the right indicates μ_H at which α transforms to β at 200 C.

Make sure to perform a careful analysis to determine the (qualitative) dependence of the transition temperature from α to β on chemical potential. In your analysis, you only need to consider configurational entropy and you can assume an ideal solution entropy.

8.

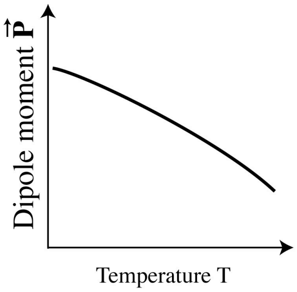
A thin film is epitaxially grown on a large substrate. The epitaxial growth constrains the lattice parameter of the film to be the same as the lattice parameter of the substrate. The film+substrate is kept in an environment at constant temperature T and pressure P. In addition, an electric field $\vec{E}$ is imposed across the film (along the z-axis).

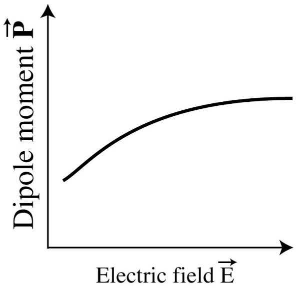
You may assume the thickness of the substrate is so much larger than the thickness of the film that the substrate has a fixed lattice parameter. The z direction is perpendicular to the film. The x and y axes are in the plane of the film. **You may neglect surface and interface effects of the film.**

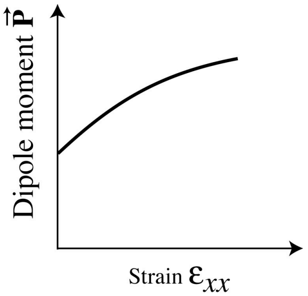


a) Write down the thermodynamic state variables *of the film* that are controlled experimentally.
b) Write down an expression for the characteristic potential of the film under these boundary conditions.
c) Write down the equations of state for the film.

The following measurements of the electric dipole moment $\vec{\mathrm{P}}$ have been made as a function of temperature, T, electric field $\vec{E}$ and strain ε_{xx}.







The film is under tensile stress along the x direction. You are worried that the film may crack as the electric field, $\vec{E}$, is increased due to the possibility that the internal stress within the film, σ_{xx}, may increase above a critical fracture stress. Based on the measurements made above, should you be worried about cracks as a result of increasing electric fields? Explain your answer.

9.

A fuel cell generates electricity by separating electrons and protons of a fuel at the anode side, forcing the electrons to travel through a circuit, to recombine on the cathode side. On the cathode side in a PEM fuel cell, oxygen gas, protons and electrons are combined to form water. This reaction is catalyzed by platinum and requires oxygen to absorb on the platinum surface.

We would like to model oxygen coverage (O) on a fuel cell platinum catalyst at constant temperature T.

Approximate the platinum catalyst system with a two-dimensional surface lattice with M sites, in contact with oxygen gas. Each site can be either occupied or empty with a single absorbed oxygen atom. The absorbed O has a binding energy $-\varepsilon$ and we neglect any interaction between the oxygen atoms.

a) Calculate the closed form *grand canonical* partition function of the system as a function of the relevant thermodynamic variables.

b) Calculate the characteristic potential of the system.

c) Calculate the average number of adsorbed oxygen atoms N as a function of the temperature, lattice sites M and oxygen chemical potential μ.

Assume that the oxygen gas is an ideal gas at some pressure P and at the same temperature T as the surface. Calculate the fraction N/M of adsorbed oxygen atoms as a function of the pressure P of the ideal gas and the temperature T of the system.

Structure of Materials **Code_______**

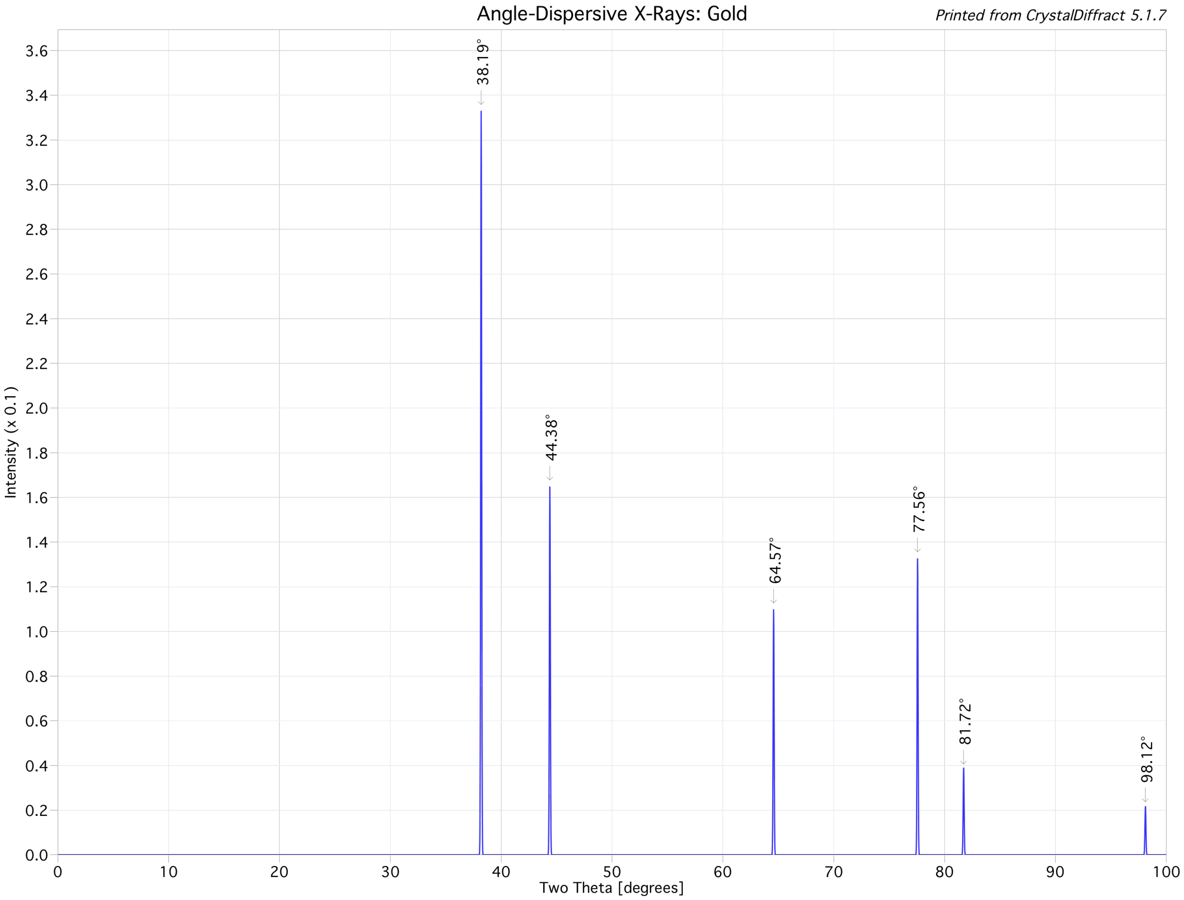
13.

The following x-ray diffraction pattern (θ-2θ) is from a cubic crystal. The 2θ values of all peaks between 0 and 100° are given. The relative intensities of peaks can be determined from the pattern. (λ=1.54Å)

(a) Determine the type of this crystal structure (i.e. simple cubic, bcc, or fcc).

(b) Determine the lattice constant of the crystal.

(c) Index all peaks in the plot.



14.

How would you distinguish between TEM image features below? Why does your method work?

a) Moirè fringes and wedge thickness fringes.
b) Bend contours and dislocation arrays.
c) Moirè fringes and dislocation arrays.

Note: Moirè fringes are caused by the overlap of two crystals with different lattice constants and/or different lattice orientations. They are sensitive to the orientation of specimen.

15.

A film of $SrRuO_3$ is grown epitaxially on a smooth (001) $SrTiO_3$ substrate. How many twinning variants (elastic domains) do you expect in the $SrRuO_3$ film at room temperature? If the film has a multiple domain structure, do all domains have the same volume fraction in the film? What will be your answers to the above questions if a $PbTiO_3$ film grows epitaxially on (001) $SrTiO_3$? (All films were grown at 700 °C.)

- At room temperature (and above) $SrTiO_3$ has a cubic perovskite structure with the space group of $Pm\bar{3}m$ and lattice constant a=3.905 Å.
- $PbTiO_3$ is a perovskite with a cubic structure above 490 °C (the Curie temperature). Below this temperature, $PbTiO_3$ is ferroelectric with a tetragonal unit cell, having lattice constants a=3.904 Å and c=4.152 Å at room temperature.
- $SrRuO_3$ is also a cubic perovskite at temperatures higher than 600 °C. It has a pseudo-cubic perovskite structure after cooling through 600 °C. At room temperature, it has the symmetry of *Pbnm* (space group no. 62) and lattice parameters a=5.5670 Å, b=5.5304 Å, and c=7.8446 Å.