Department of Materials Science and Engineering

DOCTORAL WRITTEN EXAM
May 17, 2013

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. Extra answer sheets are on the table if you need them.

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. This is for anonymity.

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 Patti in rm. 2146 Dow 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.

The valence and conduction band structure of a hypothetical semiconductor are given respectively by $E_v(k) = B_v \cos(ka)$ and $E_c(k) = A_c + B_c \cos(ka)$, where $A_c = 11\,\text{eV}$, $B_c = 4\,\text{eV}$, $B_v = 5\,\text{eV}$, and $a = 5\,\text{Å}$. The dielectric constant of the semiconductor is $\varepsilon = 10$. The electron scattering time is 11 fs

a) Plot the band structure. What is the value of the band gap? Is this a good light-emitting semiconductor? Explain why or why not.
b) What are the values of the electron and hole effective masses at the conduction band minimum and valence band maximum, respectively?
c) If donor atoms are added, what is the donor binding energy?
d) If all donor atoms are fully ionized at room temperature, each donor atom contributes one electron to the conduction band, and the donor concentration is 10^{19} cm^{-3}, what is the resistivity of the doped semiconductor?

2.

Spectrolab makes a GaAs/Ge single junction solar cell that has an open circuit voltage, V_{OC} = 1.025 V, and a short-circuit current, J_{SC} = 30.5 mA/cm^2, under illumination by AMO (1366.1 W/m^2)
Ideal Diode Equation: $I = I_o\ [\exp(qV/kT)-1]$

(a) Assuming the cell obeys the ideal diode equation, find J_0
(b) Calculate the maximum power a 1 m^2 array of these cells could deliver to a resistive load.
(c) Calculate the load resistance needed to obtain maximum power, and sketch the resulting circuit.
(d) What is the efficiency of this cell?

3.

Ferromagnetism:
Metallic cobalt (Co) has a density of 8.9 x 10^3 kg/m^3 and its molar mass is 0.059 kg/mol.
(a) If cobalt has one unpaired spin per atom and perfect spin alignment, compute the maximum magnetization.
(b) If instead cobalt consists of entirely Co^{2+} ions, each of which has seven 3d electrons, determine the net magnetic dipole moment per Co^{2+} ion.
(c) Compare the results from (a) and (b) with that of the observed maximum magnetization of ~1.4 x 10^6 A/m.
(d) Use (a) –(c) to determine the number of unpaired spins per Co atom.

4.

A titanium alloy has the following properties:
Yield strength is 1100MPa
Ultimate tensile strength is 1200MPa
Modulus of elasticity is 110GPa
Endurance limit is 550MPa
Fracture toughness is 50MPa-$\sqrt{m}$
Fatigue crack growth constants are m=3 and C= $1.6\text{x}10^{-10}$ [m/cycle/(MPa-$\sqrt{m})^3$]

a) A bar of this alloy is subjected to loading such that one principal stress is 800 MPa in tension and the other principal stresses are equivalent to each other and equal to 400MPa in compression. Provide a sketch of the Mohr's circle for this stress state. Would you expect this bar to yield? Justify your answer with a calculation.

b) A 25mm diameter rod of this alloy is subjected to a static load of 245kN and a cyclic alternating stress of 120kN. Would you expect the rod to fail by fatigue?
Justify your answer with a calculation.

c) A crack 10mm in total length is discovered in the center of a very wide plate of this material loaded under a cyclic stress range of 80MPa and R=0. Use a calculation to estimate the final crack length and the number of load cycles at which the plate will fail. You may assume that when the plate fails the crack is very small relative to the total plate width.

5.

You are designing a new, strong copper-zirconium alloy with a goal of achieving a yield strength of 400MPa at room temperature in a polycrystalline material. In addition to the Pierel's stress, two mechanisms are available in this alloy, strengthening due to cold working and precipitation hardening. In the following sections, estimate the strength contributions of these strengthening mechanisms and provide an estimate of the amount of cold work required to achieve the desired strength.

a) To determine the inherent resistance of the Cu lattice to dislocation glide a 2 mm diameter single crystal of copper is prepared and tested in tension. The tensile axis of the specimen is parallel to the $[\bar{1}23]$ direction of the single crystal. You measure the load at the yield point to be 6.74 N. What is the operative slip system? Use this information to calculate the critical resolved shear stress for Cu.

b) Determine the role of cold work as a means to strengthen copper. A series of tensile tests are conducted in materials containing a variety of dislocation densities. You find that with a dislocation density of 3×10^{14} m^{-2} in a cold worked sample the resolved shear stress required for flow is 100 MPa. Use this information to write an expression estimating the relationship between resolved shear stress and dislocation density.

c) Based on the literature you find that zirconium has very low solubility (~0.001 wt %) in copper at room temperature and provides essentially no solid solution strengthening. However, it does form a precipitate of Cu_9Zr_2. It is determined that the maximum strength occurs at a precipitate volume fraction of 1% of 40 nm diameter non-shearable precipitates. Estimate the strengthening contributions from precipitation hardening at this maximum strength condition. Assume that the precipitates are spherical and are distributed in a cubic pattern.

d) Now that you have an understanding of how these mechanisms contribute to strengthening, describe and show how you would attempt to achieve the yield strength, σ_o, goal of 400 MPa in a polycrystalline material. Assume that grain size effects are negligible. Provide quantitative estimates to support your choices.

6.

A thin walled spherical steel pressure vessel is used for containing pressurized liquid at a pressure of 24 MPa. It is often subjected to rough handling that can induce gouges and fatigue cracks can initiate from these gouges. The inner radius of the pressure vessel is 1m and the wall thickness is 30mm. Two steels are under consideration for this application: Steel A has a yield strength of 1600 MPa and a K_Q of 25 MPa$\sqrt{\text{m}}$ (in 30mm thick samples), Steel B has a yield strength of 800 MPa and a K_Q of 180 MPa$\sqrt{\text{m}}$ (in 30mm thick samples).

a) What design philosophy should be used in selecting the steel?
b) Calculate the critical crack length (total crack length) for each steel.
c) Recommend a steel for this application and provide a rationale for your selection.

The following may be helpful for your calculations:

$\sigma_t = pr_i/2t$ where σ_t is the hoop stress, p is the pressure, r_i is the inner radius of the vessel and t is the thickness

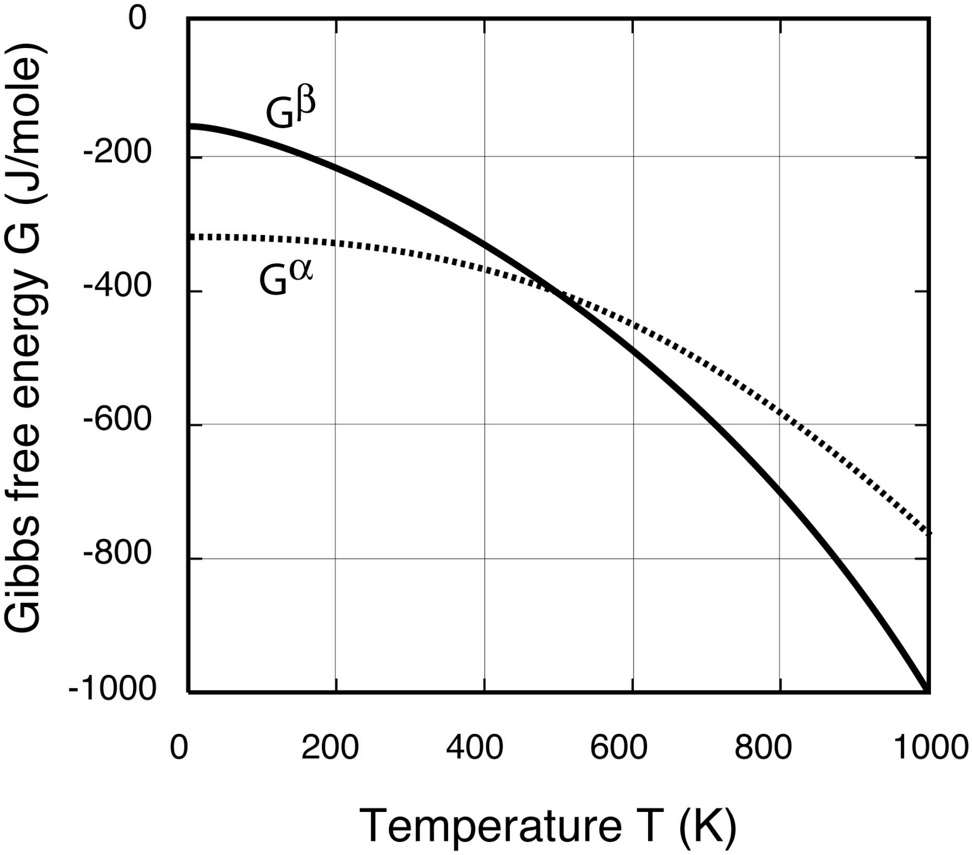
$K_I = 0.722\sigma_{applied}(\pi a)^{0.5}$ – for a half-circular surface crack of radius, a (this relationship is only valid for $a/t < 0.4$)

7.

Given the fact that calorimetry experiments (measuring the heat flow as function of temperature) and dilatometry (measuring thermal expansion) are relatively easy, but measuring properties at variable pressure is <u>not</u> easy, how would you determine the variation of heat capacity C_p with pressure for a material? Write the pressure dependence of C_p (at constant temperature) in terms of easy to measure quantities.

8.

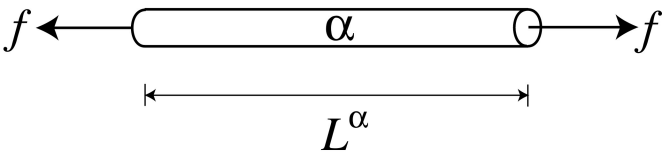
The figure below illustrates the free energies of two crystal structures, α and β, of a single component system as a function of temperature.

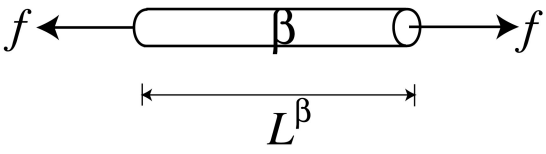


a) Use the graph to estimate the entropy change $\Delta S^{\alpha\rightarrow\beta} = S^\beta - S^\alpha$ of the transformation at T_{tr}.
b) Estimate the enthalpy change $\Delta H^{\alpha\rightarrow\beta} = H^\beta - H^\alpha$ of the transformation at T_{tr}.
c) What is the change in entropy of the universe $\Delta S^{universe}$ at T_{tr}.
d) Which of the two phases has stiffer bonds between the atoms (you can assume that the two phases are insulators with negligible electronic entropy)?

9.

A rod is made of a material that undergoes a martensitic phase transition. At low temperature, the material is in the α phase while at high temperature it is in the β phase. The rod has a substantially larger length in the α phase than in the β phase. The rod is coated with a thermally insulating material that prevents any heat exchange between the rod and the environment.





Assume that a force is applied to the ends of the rod (you can neglect PV work). You can also assume that any changes in force occur very slowly such that the change of state can be approximated as occurring reversibly. The rod starts in the β phase and is stretched above the transition force, f^*, above which β transforms to α under the conditions of thermal insulation and very slow stretching. In the actual experiment, though, the rod remains metastable in the β phase for a sufficiently long time to allow a change in boundary conditions whereby the length of the rod in the final stretched state is held clamped at a fixed value. After clamping the rod (with metastable β) it ultimately transforms to a two-phase coexistence between α and β.

a) What happens to the entropy of the rod (briefly justify your answer)?
b) Derive equilibrium criteria for this two-phase equilibrium (that is what happens to the temperatures and forces within the different phases in the rod)?
c) Will the force in the rod increase or decrease after the transformation occurs (explain your answer)?

Kinetics and Phase Transformations

Code ________

10. no one taking this area

Kinetics and Phase Transformations **Code _________**

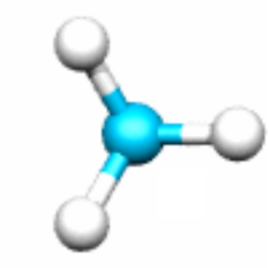
11. no one taking this area

Kinetics and Phase Transformations **Code________**

12. no one taking this area

13.

a) Find the crystal system and Bravais lattice type of space groups $R\bar{3}m$ and $Pm\bar{3}$.
b) Does the point group *mm2* consist of a center of symmetry?
c) Explain the locations of mirror planes in *Pmm2*.
d) Find all symmetry elements of the NH_3 molecule (ammonia) and find its corresponding point group. (Note that the N atom is located below the plane formed by three H atoms.)



14.

A ternary phase has the following atoms in a cubic unit cell: A at (0, 0, 0), B at (½, ½ , 0) and C at (½, 0, ½), (0, ½, ½). Calculate the following structure factors in terms of atomic scattering factors f_A, f_B and f_C:

(**a**) (001) and (002), and

(**b**) (100) and (200).

15.

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 (simple cubic, bcc, or fcc).

(b) Determine the lattice constant of the crystal.

(c) Index all peaks in the plot.