

Department of Materials Science and Engineering

**DOCTORAL WRITTEN EXAM
May 21, 2009**

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 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. _____

4.

Consider a face centered cubic material with tensile axes aligned along $\langle 001 \rangle$, $\langle 011 \rangle$ and $\langle 111 \rangle$ type of directions – 3 separate cases. How many slip systems operate for these respective cases? Explain each situation in detail.

5.

A material has true stress-true strain curve given by the equation $\sigma = k \epsilon^n$, where k and n are constants.

- a) By satisfying the condition for maximum load in a tensile test (i.e. at the onset of necking), determine the extent of uniform strain in the sample. Show the steps in your work.
- b) If the true fracture stress in tension is σ_F , determine the cross sectional area of the sample at fracture in terms of original cross-sectional area and the constants in the equation.
- c) If n is a linear function of true strain rather than a constant, would the uniform strain increase or decrease? Provide your answer by using a simple mathematical form.

6.

A copper single crystal (f.c.c.) is stressed uniaxially along [111] direction.

- a) When the stress reaches 100 MPa what will be the normal stress component along [100], [010] and [001] directions?
- b) Given the values of compliance constants for copper as $s_{11} = 1.5 \times 10^{-11} \text{Pa}^{-1}$, $s_{12} = -0.63 \times 10^{-11} \text{Pa}^{-1}$ and $s_{44} = 1.33 \times 10^{-11} \text{Pa}^{-1}$, what will be the value of normal strain in those directions?

7.

A rod, having length L_o in the unstressed state at temperature T_o , is elongated to a length L_l at temperature T_o .

Assume the rod is elongated very slowly by steadily increasing the force on the ends to f_l such the change of state can be approximated as a reversible one.

- a) Schematically sketch the change of state in an f - L diagram.
- b) How much work is applied to the rod to isothermally extend it from L_o at zero force to L_l at force f_l ?
- c) How much heat is exchanged between the rod and the environment during this change of state?

Assume the rod is elongated by attaching a weight to one end with mass M such that $Mg=f_l$.

- d) Is this change of state reversible?
- e) How much work is applied to the rod by the environment once the rod has equilibrated with the environment at T_o ?
- f) How much heat is exchanged between the rod and the environment during this change of state?

You may find the following relation between state variables useful:

$$L = L_o + \alpha(T - T_o) + \beta f \quad \text{where } \alpha \text{ and } \beta \text{ are constants.}$$

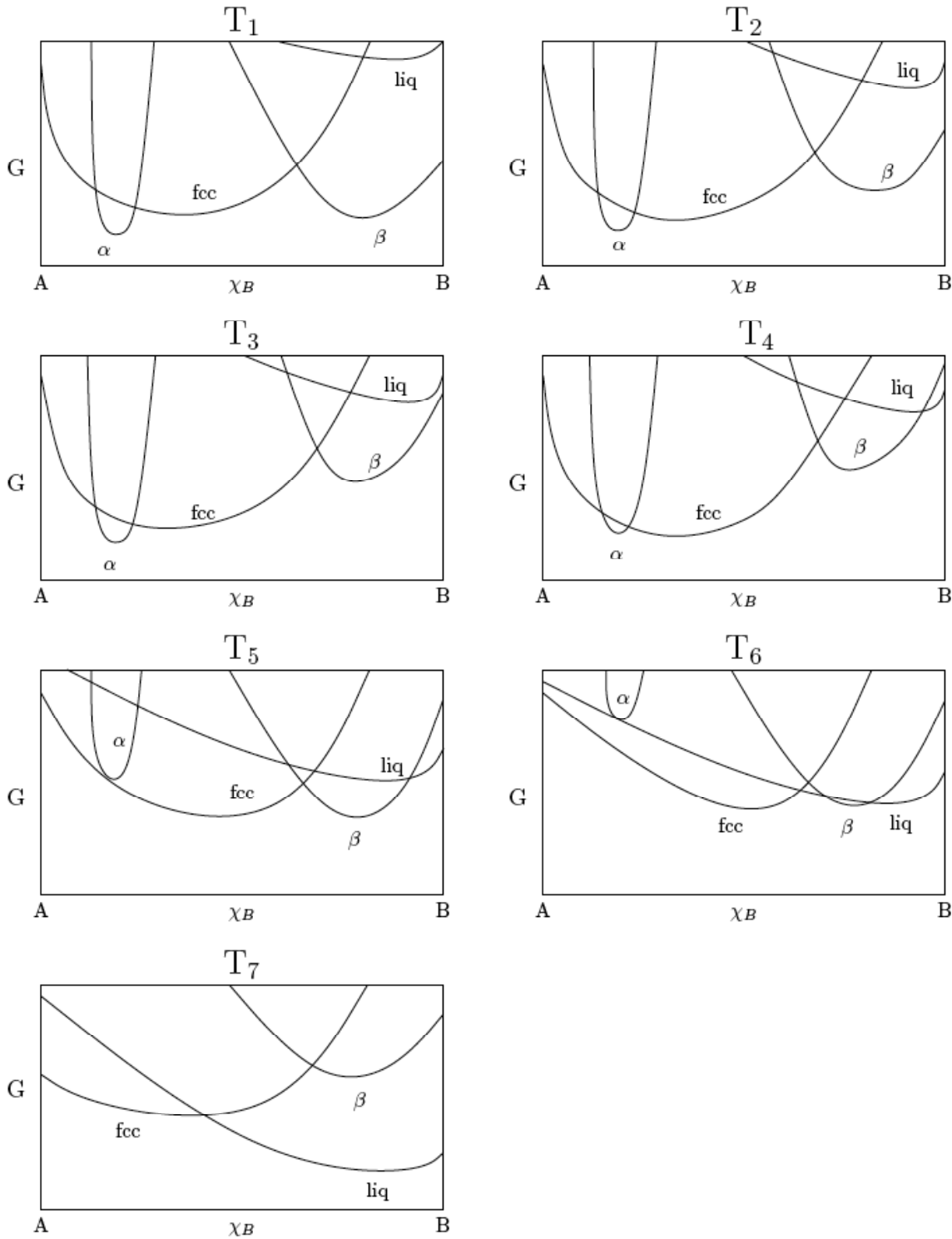
8.

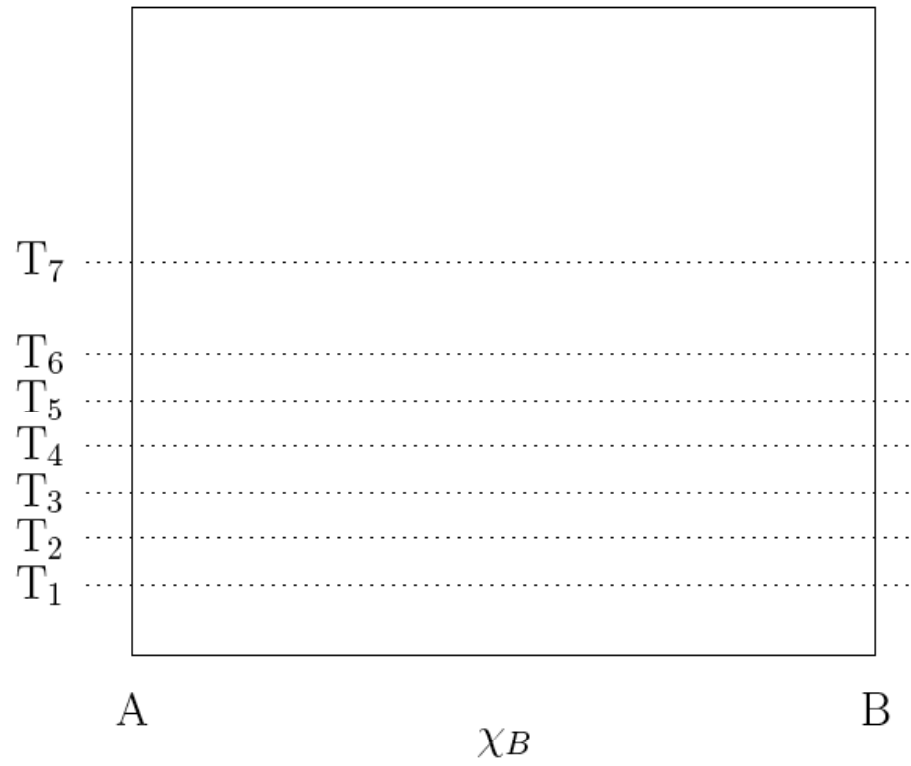
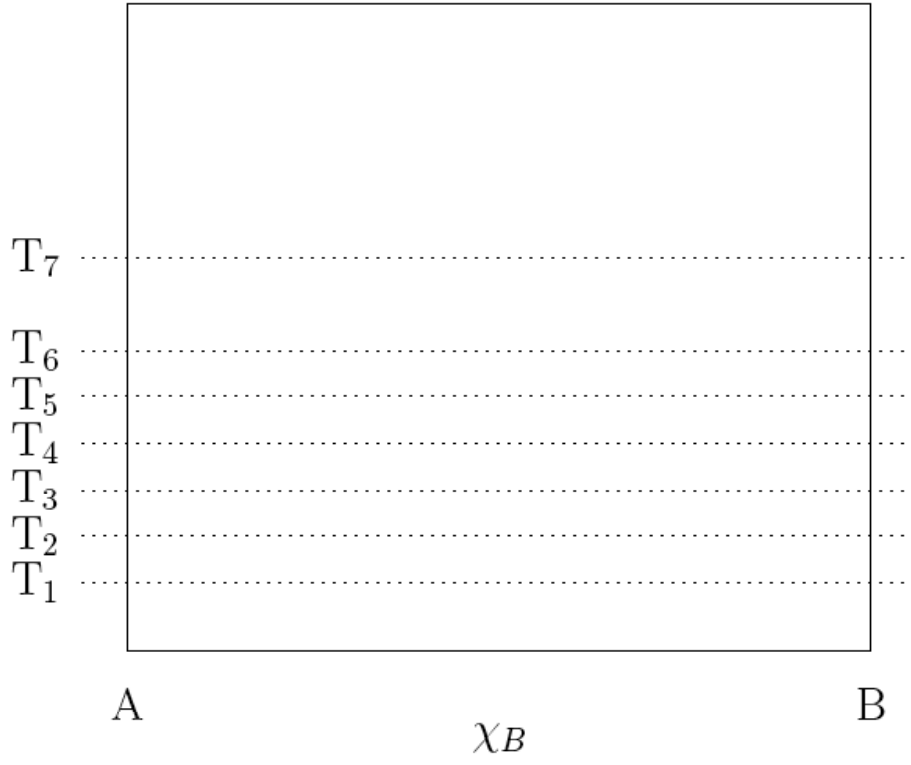
A single component fcc crystal is susceptible to the formation of Frenkel defects, whereby a substitutional atom of the crystal fills an interstitial site, leaving behind a vacancy. Assume that the interstitial atoms only fill octahedral interstitial sites of the crystal (the number of octahedral interstitial sites is equal to the number of fcc substitutional sites). The energy of the perfect crystal is E_0 and the energy cost of forming a Frenkel defect is ε . You can assume that the energy of the crystal is independent of the arrangement of vacancies and interstitial sites.

- a) Let n denote the number of Frenkel defects (i.e. number of vacancies and number of interstitials). Determine the partition function of the crystal at constant T and V assuming that the number of Frenkel defects n is constant.
- b) Use the result of (a) to derive an expression for the free energy of the crystal containing n Frenkel defects.
- c) Derive an expression for the configurational entropy of the crystal when n Frenkel defects are present.
- d) The number of Frenkel defects in a crystal cannot be controlled experimentally. Write an equilibrium criterion that will allow us to determine the number of Frenkel defects in thermal equilibrium.
- e) If interactions between the interstitial and the vacancy of the Frenkel defect were important, would the configurational entropy of the crystal be larger or smaller than that determined in part (c)? Why?

9.

A group of thermo students have solved the equations of quantum mechanics and statistical mechanics to obtain the Gibbs free energy for the A-B system. They are shown below as a function of composition at seven different temperatures. Please draw the phase diagram on the next page. Clearly indicate the phase diagram to be graded.





10.

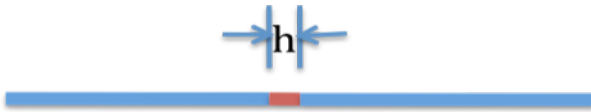
The melting point of gold is $T_m=1062^{\circ}\text{C}$; the enthalpy of formation of a single vacancy is 5.2 kJ/mole and the entropy of formation is $S/k=1$. The binding energy for a divacancy is 0.9 kJ/mol.

- a) If one measured the $\Delta a/a$ (a is the lattice parameter) and $\Delta L/L$ (L is the sample dimension), how could the vacancy concentration be determined from knowledge of this information?
- b) If your intent is to measure the single vacancy concentration only, what is your margin of error at $T=T_m/10$?
- c) Write down an expression for the self diffusion coefficient, D_s , of single vacancies.
- d) Make your best estimate of the magnitude of the self diffusion coefficient of gold at $T=T_m/2$. Please state any assumptions you make about the magnitude of any parameters. The parameters must be of reasonable magnitude.
- e) Having calculated D_s , calculate a value for the tracer diffusion coefficient.

11.

The diffusion of particles from a point source, of initial concentration c_0 (an mass M) occurs via Brownian motion.

- Briefly explain Brownian motion
- Write down an expression describing the concentration of the particles, $c(x, t)$, at distance x from the origin at time t .
- Determine the average concentration of the particles at time t .
- What is the probability that the particle will be at location x , at time t .
- What is the average displacement of the particle, $\langle x \rangle$? Show your answer explicitly.
- Consider now that the particles are initially confined to a region of the sample of length h . Write down an expression for the concentration profile $C(x, t)$.



- Write down an expression describing the total amount of material that diffused out of the region after time t .

12.

The diffusion coefficient of polystyrene of degree of polymerization $N=1000$ (molecular weight of the monomer is $M_0=104$) is $D_{\text{REP}}=10^{-13}$ cm²/s at $T=180^\circ\text{C}$. Assume that the plateau modulus is 2×10^6 dynes/cm, $R_g=10$ nm, $M_c=30,000$ g/mol, $M_e=18000$ g/mole and density is $\rho=1$ g/cm³, where k is the Boltzmann coefficient, T is the temperature and ζ_0 is the monomer friction coefficient.

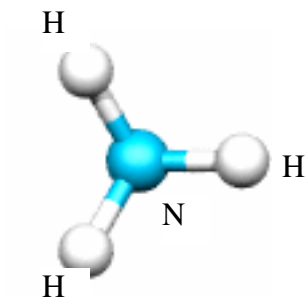
- a) Determine the viscosity at $T=180^\circ\text{C}$
- b) If you considered a polymer such as polymethyl methacrylate (PMMA), of the same molecular weight and the same temperature, would you expect the viscosity to be larger or smaller? Explain
- c) If the WLF coefficients are $C_1=12$ and $c_2=50$ at a reference temperature of $T=100^\circ\text{C}$, what is the viscosity at 120°C .
- d) Explain the reason the log of the temperature dependence of the diffusion coefficient of an amorphous polymer is the same as that of the log of the inverse viscosity ($\log \eta^{-1}$).
- e) Why is the temperature dependence of diffusion of polymers not Arrhenius? Explain.

13.

- a) Draw the unit cell of the reciprocal lattice of a body-centered cubic (bcc) crystal lattice.
- b) Calculate the angle between the [110] direction and the (111) plane in a cubic crystal.
- c) Calculate the angle between the [110] direction and the (111) plane in an orthorhombic crystal
($a = 0.5400$ nm, $b = 5.500$ nm, and $c = 0.7800$ nm).
- d) Which of the following configuration has the highest packing efficiency: BCC, HCP, FCC, and simple cubic?

14.

- Find the crystal system and Bravais lattice type of space groups $R\bar{3}m$ and $Pm\bar{3}$.
- Does the point group $mm2$ consist of a center of symmetry?
- Explain the locations of mirror planes in $Pmm2$.
- 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.)

(20 points)

15.

Figure 1 (below) is an electron diffraction pattern from a *f.c.c.* single crystal. The diffraction pattern was taken using camera length $L=716\text{mm}$, electron energy 120keV (wavelength = 0.0335\AA). Please find the indices of reflections indicated by A, B, and C, and find the zone axis of this diffraction pattern.

$OA=13.3\text{mm}$, $OB=OC=11.43\text{mm}$, $\angle AOB = 54.74^\circ$, $\angle BOC = 70.53^\circ$. (30 pts)

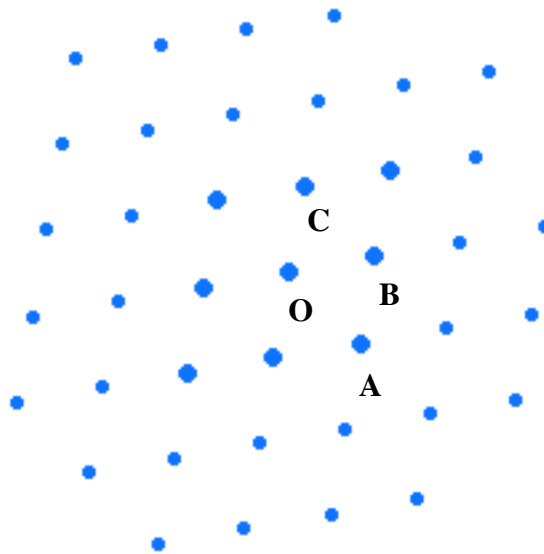


Figure 1