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 24, 2013

Department of Materials Science and Engineering

DOCTORAL WRITTEN EXAM
January 24, 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. 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:	Advanced Mechanical Behavior:
1. _____	4. _____
2. _____	5. _____
3. _____	6. _____

Advanced Thermodynamics Of Materials	Kinetics and Phase Transformations	Structure of Materials
7. _____	10._____	13._____
8. _____	11._____	14._____
9. _____	12._____	15._____

Materials Physics and Chemistry **Code_____**

1. Drude Theory

The Drude Theory assumes that a metal is composed of stationary ions with valence electrons that move in a manner similar to that of the molecules in an ideal gas.

(a) Determine the rms velocity of a conduction electron in a metal at T=295K.
(b) Assuming that the electron mean free path is ~1nm, calculate the average time between collisions.
(c) Use the values in (a) and (b) to determine the mobility and drift velocity of an electron in a metal in an electric field of 10 V/m at 295K.
(d) Explain why the drift velocity is much smaller than the rms velocity calculated in (a)

Materials Physics and Chemistry **Code_____**

2. Radiation from the Sun

radius of the sun = 6.96 x 10^5 km
earth-sun separation (center-to-center) = 1.49 x 10^11 m
radius of the earth = 6.37 x 10^6 m

a) Estimate the intensity of solar radiation on the Earth's surface.
Assume that the Sun is a perfect blackbody, consider normal incidence only, ignore the effect of the atmosphere, and express the answer in units of W/m2.
b) What is the total solar power incident on the Earth?
c) Assuming that the Earth is a perfect blackbody that reemits the energy absorbed from the Sun, estimate the temperature of the Earth.
d) How does the answer of part (c) change if you take into account the 30% reflectivity of the atmosphere?

3. Band Theory of electrical conduction

In this question, we estimate the proportion of valence electrons that participate in electrical conduction in a Au metal film at 300K, using Fermi-Dirac statistics, and the following parameters:

Fermi Energy = 5.51 eV
Electron concentration = 5.90×10^{22} /cm^3

(a) Determine the energy which corresponds to an occupation probability of f=0.7
(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 1D? Show your work.

4. Complete both parts a) and b):

a) The lattice parameters of Ni and Ni_3Al are 3.520×10^{-10}m and 3.567×10^{-10}m, respectively. The addition of Cr to a Ni-Ni_3Al superalloy increases the lattice parameter of the Ni matrix to 3.525×10^{-10}m. Calculate the fractional change in alloy strength associated with the Cr addition, assuming all other factors are unchanged. Provide a rationale for your calculations and describe the result.

b) In FCC materials the stacking fault energy is an important parameter for plastic deformation. Describe the impact that increasing the stacking fault energy has on the stacking fault width, on cross slip and on work hardening.

Advanced Mechanical Behavior **Code_____**

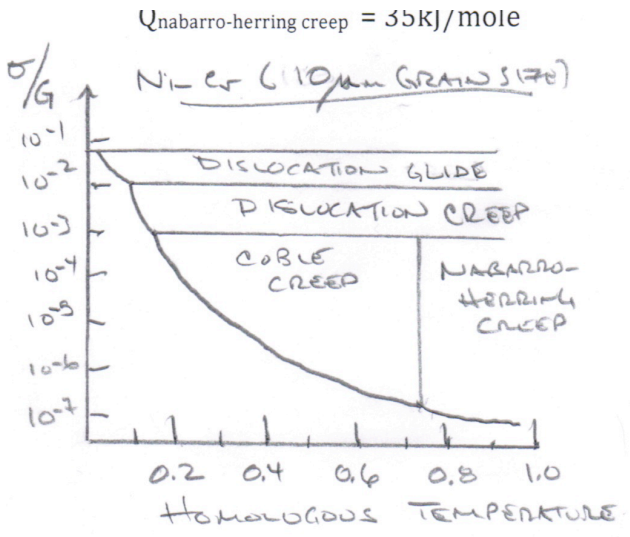
5. Complete both parts a) and b):

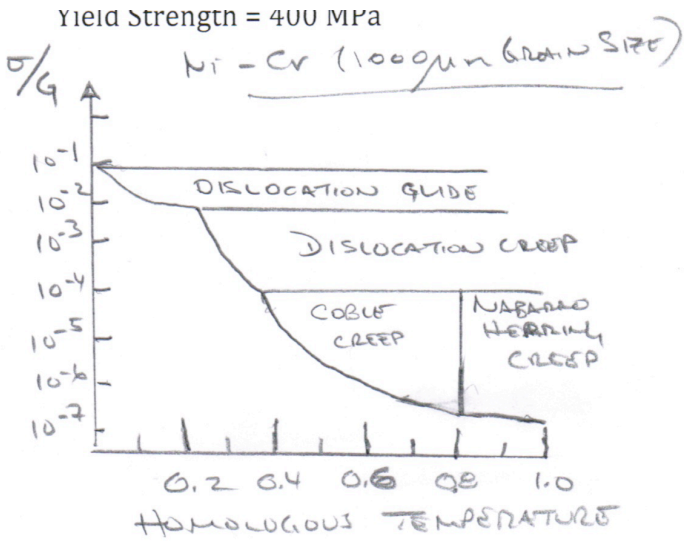
a) For a certain high-temperature steel, creep rupture was reported after 4100 hrs at 680°C when subjected to a stress level of 270 MPa. If the same stress were applied at 725°C, how long would the sample be expected to last? State any assumptions you must make to allow you to make this determination.

b) A heat treating furnace element is manufactured from a nickel-chrome alloy and is subjected to a sustained stress of 1 MPa at a temperature of 727°C. Creep mechanism maps for this alloy are shown below. An initial calculation indicates that the steady state creep strain rate will be $1x10^{-8}$/sec, however the design requires a steady state creep strain rate of $1x10^{-9}$/sec. The material has been processed to provide a grain size of 100μm. It has been proposed that the component be processed to change the grain size to achieve the required steady state creep rate. Describe if this would be an effective strategy for improving the creep resistance of the furnace elements and, if so, why and what grain size would be required. If you conclude that this would not be an effective strategy, support your conclusion and provide an alternate solution. In either case, show calculations to support your conclusions.

R=8.31 J/mole-K
$Q_{self\ diffusion}$ = 375kJ/mole
$Q_{coble\ creep}$ = 75kJ/mole
$Q_{nabarro\text{-}herring\ creep}$ = 35kJ/mole

Young' Modulus = 205GPa
Shear Modulus= 79GPa
Alloy Melting Point = 1453 °C
Yield Strength = 400 MPa





Advanced Mechanical Behavior **Code_____**

6. Complete both parts a) and b):

a) Assuming a cracked structure is subjected to a constant cyclic stress, $\Delta\sigma$, derive a general, analytical (closed form) expression for the number of cycles to propagate an initial crack, of length a_o, to final fracture at crack length, a_f. Please provide a rationale for all assumptions used.

b) A semi-circular crack of depth a=0.25cm is discovered on the inner diameter of an aluminum alloy pressure vessel. The crack is oriented along a line parallel to the cylinder axis. The pressure vessel has a length of 100cm; outer diameter of 10cm and an inner diameter of 7cm. If the cylinder is repeatedly pressurized from 0 MPa to 75MPa, use the expression in part a) to estimate the cyclic life of the pressure vessel.

The material obeys a Paris-Law relationship with $c=5x10^{-15}$ (the units of the relationship are in m/cycle and MPa-$\sqrt{m}$) and the crack growth rate has been determined to be proportional to the square of the crack tip plastic zone size.

Show and justify all assumptions. For any stress intensity calculation that may be required, you may assume that F(a/b)=1.0 and finite width corrections may be neglected.

The following information may be useful.
The fracture toughness of this aluminum alloy is 30 MPa-$\sqrt{m}$;
the yield strength of this aluminum is 400MPa;
$\sigma_{hoop} = PD/2t$

7. A surface with M-sites can adsorb oxygen atoms. The energy of adsorption is ε_o. The adsorption sites are far enough apart from each other such interactions between them can be neglected. The adsorbed oxygen atoms have a mass m and reside in a potential well with force constant f (the same value in all three directions x, y and z). The surface is in equilibrium with a gas phase of oxygen molecules at constant chemical potential μ and constant temperature T.

a) Write down the characteristic potential for the given boundary conditions
b) Derive an analytical expression for the partition function
c) Derive an expression for the equilibrium concentration of the adsorbed oxygen atoms
d) Stretching the surface isotropically in the plane of the surface results in a decrease of the force constant f of the adsorption sites. What will happen to the equilibrium concentration of adsorbed oxygen atoms if the surface is stretched (briefly explain why)?

8. You are asked to explore whether a ferroelectric material could be used to cool a micro-electronic device. The idea would be to place the ferroelectric material between charged capacitor plates such that the material is in an electric field $\vec{\mathrm{E}}$. When cooling is required, the electric field would suddenly be switched off. The hope is that the resultant relaxation of the total dipole moment $\vec{\mathrm{P}}$ would be accompanied by the absorption of heat.

Given the following relations among the thermodynamic state variables of the ferroelectric material, derive an expression for the amount of heat absorbed by the ferroelectric material after an electric field with value E_1 is suddenly switched off. The temperature T of the ferroelectric is less than T_c.

$$\vec{\mathrm{P}}\left(T,P,\vec{\mathrm{E}}\right) = A\cdot\left(T_c - T\right)^{1/2} + \chi\cdot\vec{\mathrm{E}}$$

(T_c is the ferroelectric transition temperature and A and χ are constants)

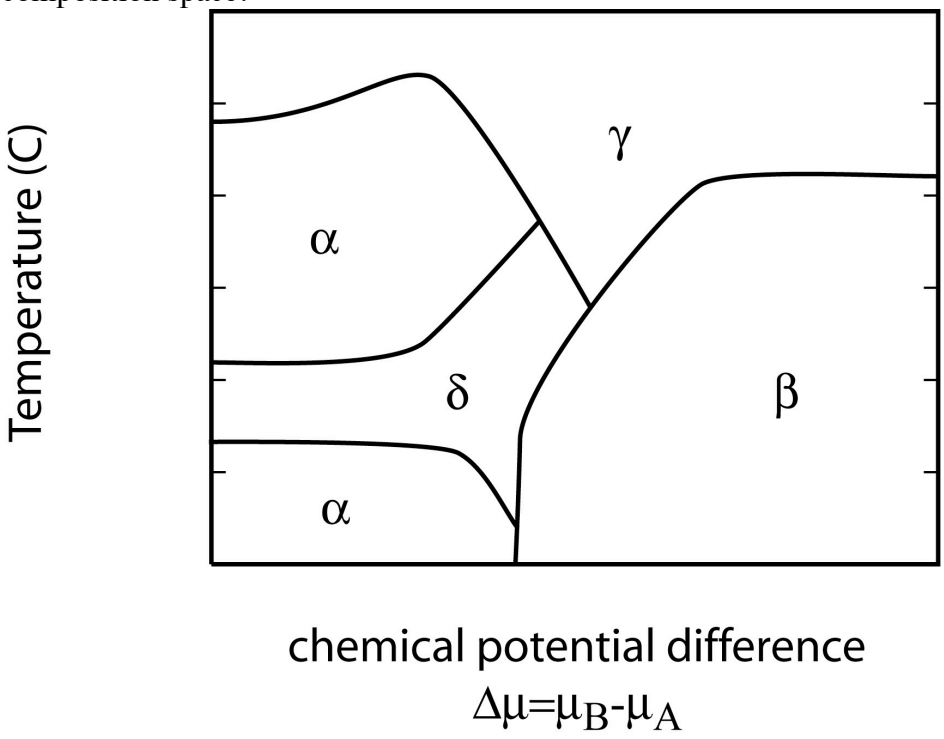
$C_{P,\vec{\mathrm{E}}}$ =constant (heat capacity)

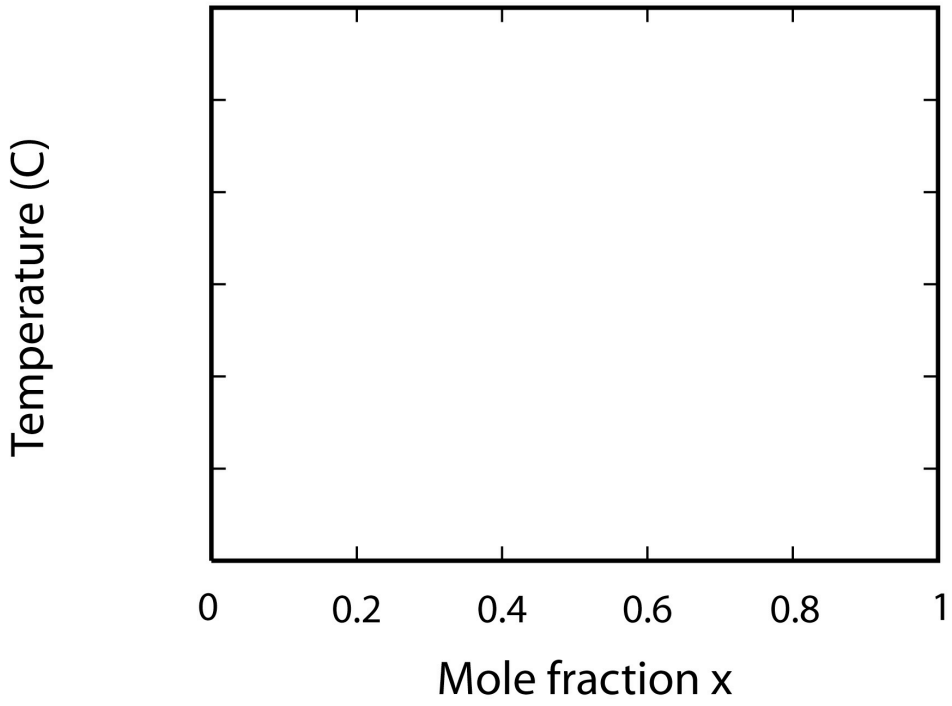
$$\beta = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{P,\vec{\mathrm{E}}} = \text{constant}$$

$$\kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{T,\vec{\mathrm{E}}} = \text{constant}$$

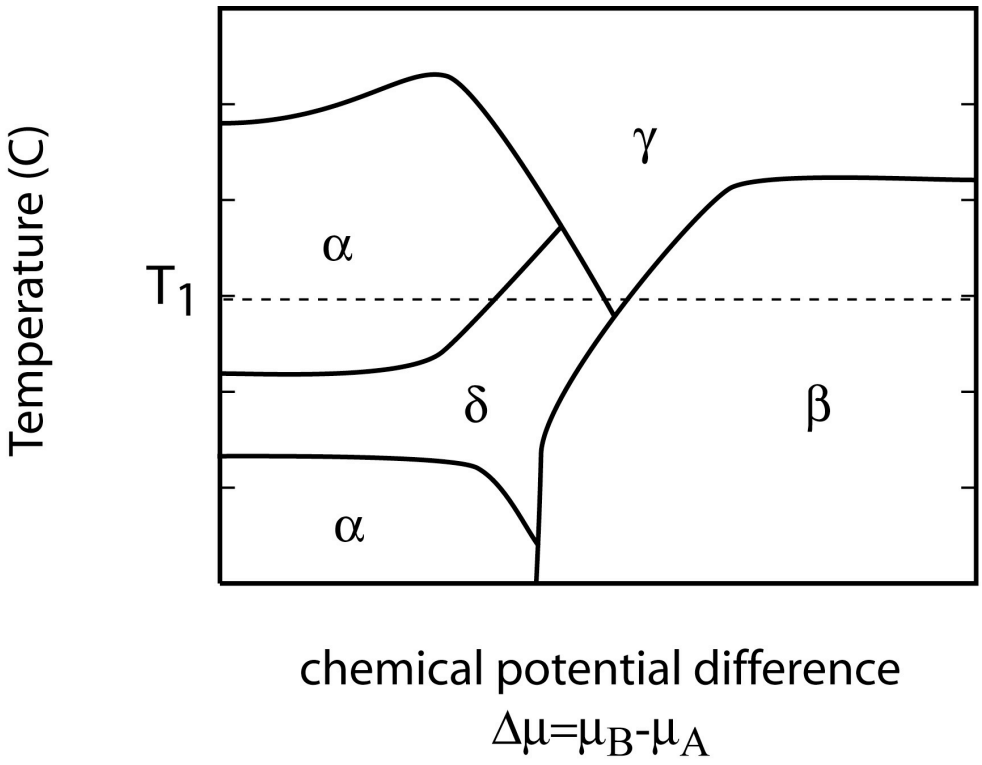
9.

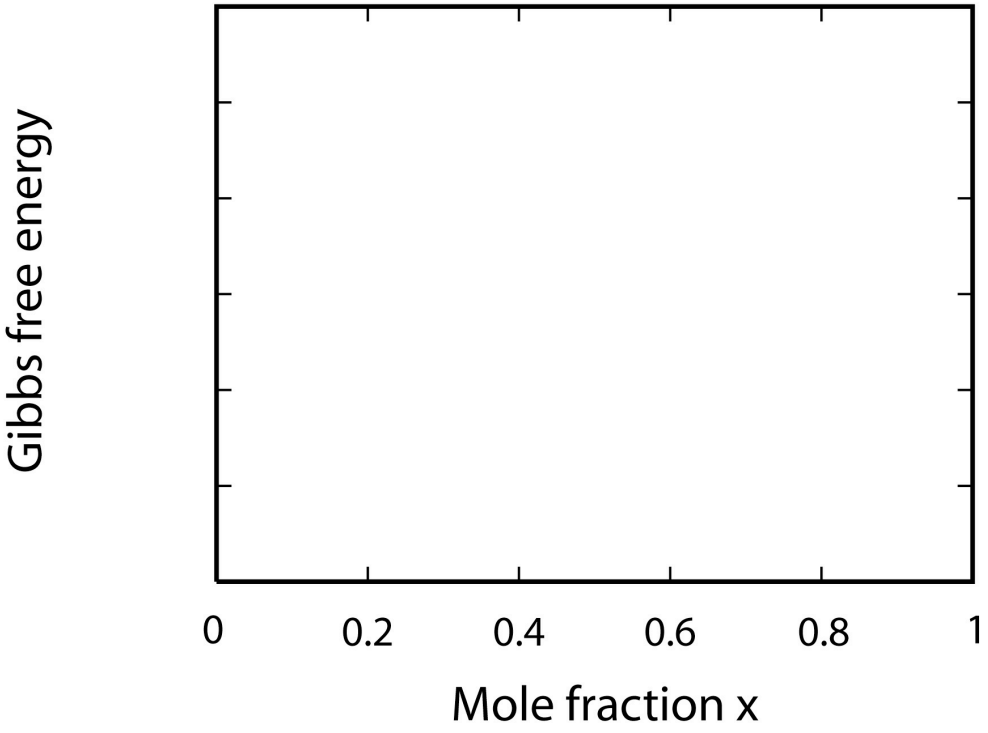
(a) For the phase diagram below, schematically draw corresponding phase diagram in temperature composition space.



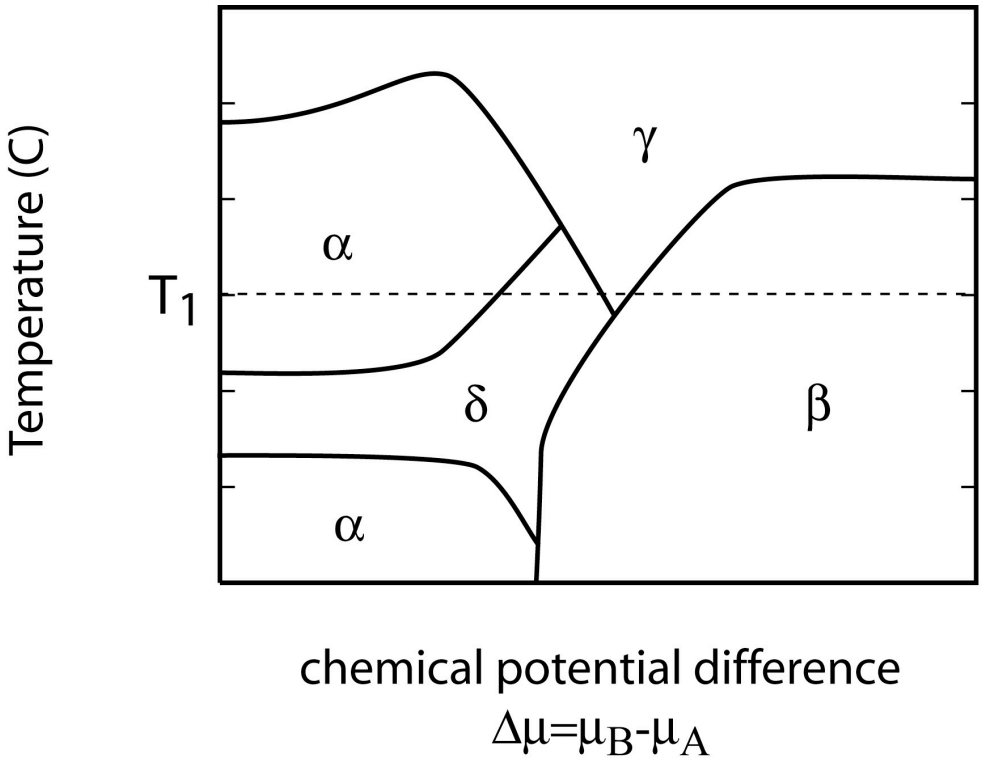


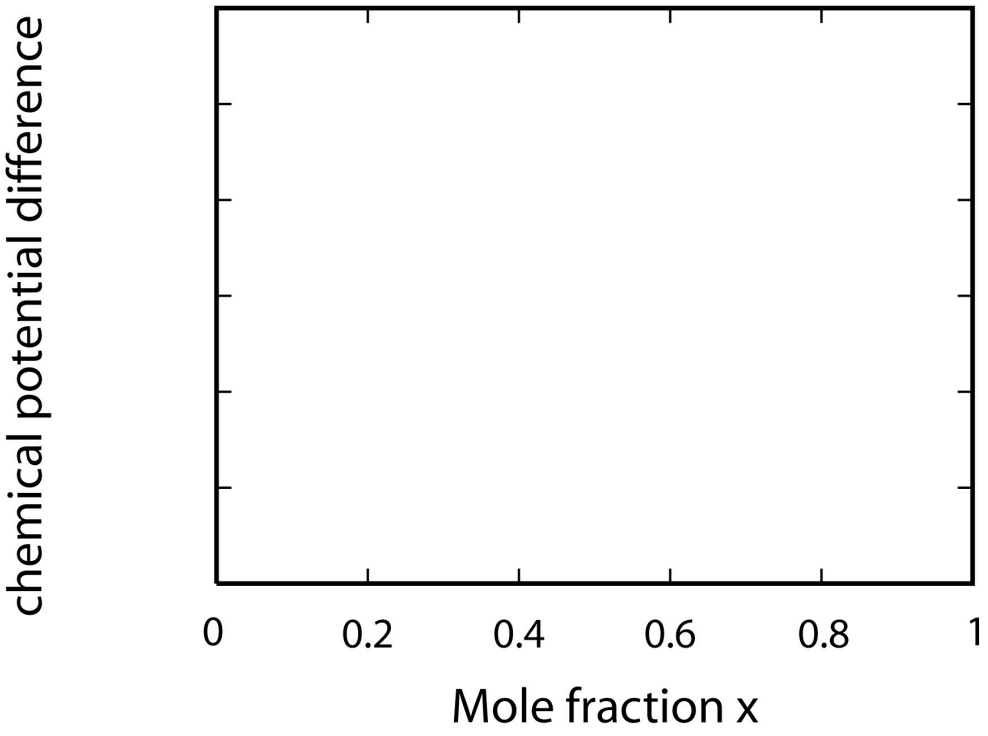
(b) Schematically draw the Gibbs free energy diagram at T_1.





(c) Schematically draw the chemical potential difference $\Delta\mu$ as a function of concentration at T_1.





10. At room temperature nitrogen gas molecules impinge upon the surface of a metal substrate, and adsorb following a Langmuir isotherm, i.e., the thickness of adsorbed nitrogen does not exceed a monolayer. Maximum surface coverage allows for 1.5 nitrogen molecules per square nanometer. Impingement leads to adsoption as long as the velocity component normal to the surface provides a kinetic energy in excess of 30 kJ/mol.

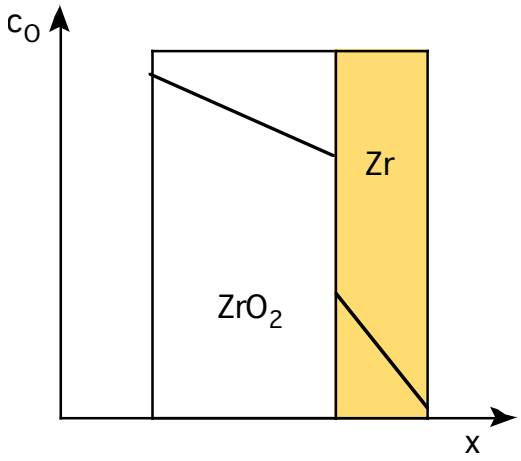
a) Use the collision rate theory to calculate the value for the reaction rate coefficient k.
b) Now consider a pristine metal surface (i.e., devoid of any adsorbed species) exposed to an atomosphere of pure nitrogen at 300 K and 10^5 Pa at time zero. Assume that the desorption rate coefficient is four times smaller than the adsorption rate coefficient. Calculate how long it takes to reach the equilibrium adsorption coverage (within 1% accuracy).

11. Consider the inter-diffusion of two species A and B. The chemical diffusion coefficient is adequately described by Darken's equation and the mixing behavior of the two components is described by the regular solution model, in which $\ln \gamma_A = (\alpha/RT) x_B^2$. The magnitude of the factor α/RT is of the order of unity; it is positive in case the system tends to phase separate and it is negative in case it tends to form a compound. At the chosen temperature, the self-diffusion coefficients of A and B are 10^{-8} cm^2/s and $2.5 \cdot 10^{-8}$ cm^2/s, respectively.

a) Determine whether diffusion of either species occurs faster in a mixture that tends to phase separate or that tends to form a compound, e.g., by comparatively evaluating the chemical diffusion coefficient at $x_B = 0.5$. Ignore correlation effects in self-diffusion.

b) Assuming that $\alpha/RT = -1$, which species migrates faster at $x_B = 0.5$, *A* or *B*?

12. Assume a thin foil of zirconium, heated to 1000K. On one side the foil is exposed to pure oxygen, on the other side to pure carbon monoxide (CO). The oxidation of Zr progresses as oxygen diffuses across the ZrO_2 layer. However, because Zr metal has a finite solubility for oxygen, the reaction at the ZrO_2/Zr interface is slowed down and comes to a halt before all Zr is oxidized.



a) Explain why.

b) What are the relative thicknesses of the ZrO_2 and Zr layers after very long time. Assume that the gas compositions on either side do not change.

For your explanations refer to the schematic above. The molecular weight of Zr is 91.22 g/mol, that of O is 16 g/mol. The density of ZrO_2 is 5.6 g/cm^3 and that of Zr is 6.49 g/cm^3. The concentration of oxygen in ZrO_2 at the ZrO_2/gas interface is 1.08 times higher than at the ZrO_2/Zr interface. The maximum solubility of oxygen in Zr is 2.5 mol%. The equilibrium concentration of oxygen in Zr at the Zr/CO(gas) interface is zero. The diffusion coefficients of O in ZrO_2 and Zr at that temperature are $2.3 \cdot 10^{-7}$ and $6.5 \cdot 10^{-6}$ cm^2/s respectively.

13.

a) Calculate the positions (2θ) of the first five reflections of a chromium powder sample (Cr, bcc, a = 3 Å) using Cu-K_α radiation (λ = 1.54 Å).

b) If the full-width-at-half-maximum of the (110) peak is 1.0 degree, what is the average size of particles in this powder?

14. The ordered $AuCu_3$ phase has the $L1_2$ structure (Au occupies the corners of the cell, whereas the Cu atoms occupy the face centers).

(a) What is the Bravais lattice of this structure?

(b) What is the Bravais Lattice of the disordered structure?

(c) Calculate the structure factor for both the disordered and ordered states of $AuCu_3$ and determine which reflections are only present in the ordered state (these are known as *superlattice reflections).*

(d) In the disordered state, the probability of finding a Au atom in the origin of the cell is 25%; in the ordered state, it is 100%. Write down similar probabilities for the Cu atoms for both types of position in the unit cell.

(e) Find an expression for the atomic scattering factor for a partially ordered state, i.e., when the probability of finding Au in the origin of the cell is given by $25\% \le p_{Au} \le 100\%$.

Structure of Materials **Code_____**

15. Figure shown below is a phase diagram of two metals A and B that are partially soluble. Draw schematics to show the characteristics of x-ray diffraction patterns (ϑ–2ϑ) of the solid solutions at H, K, L, and M, respectively. Assuming the α phase has a f.c.c. structure with a lattice constant of a = 0.4 nm, while the β phase has a simple (primitive) cubic structure with a lattice constant of a = 3.0 nm. (Assuming that the lattice constants do not depend on temperature.)