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 29, 2010

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 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 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.

Consider a one-dimensional monatomic solid with *N* atoms and $N_L(V)$ vacancies at temperature $T > 0$ *K*. Show that the fractional vacancy concentration $n_v(T) = N_L(V)/N$ is given approximately by $n_v \approx \Delta l / l_0 - \Delta a / a_0$. Here $l_0 = N a_0$ is the length of the solid at T = 0 K, and Δa is the change in the lattice constant.

2.

Metal	**Workfunction (eV)**	**Density (g/cm^3)**	**Atomic weight (g/mol)**
Li	2.49	2.7	6.94
Na	2.28	0.968	22.99
K	2.3	0.86	39.1
Rb	2.16	1.53	85.5
Cs	2.14	1.93	132.9

a) Explain the trend in the workfunction among the metals above
b) If Li is in contact with Cs, draw the resulting band structure, including the vacuum level
c) If Li is in contact with intrinsic (pure) Si ($E_g \sim 1.1$ eV) and a voltage is applied, as shown below, draw the resulting current-voltage characteristic. Explain.

3.

Qualitatively, plot the absorption spectra for the following materials:

a) Lithium and Potassium – on the same set of axes.
b) Lithium and Silicon – on the same set of axes.
c) Silicon and Germanium – on the same set of axes.
d) Silicon and GaAs – on the same set of axes.

4.

Strain gauges mounted on the free surface of a piece of steel ($E = 205$ GPa, $\nu = 0.29$) indicate strains of $\varepsilon_x = -.00042$, $\varepsilon_y = .0007$, $\gamma_{xy} = 0.00037$

a) Calculate the principal strains.
b) Use Hooke's law to find principal stresses form principal strains

5.

a) Calculate Young's Modulus for an iron crystal when tension is applied along a <122> direction

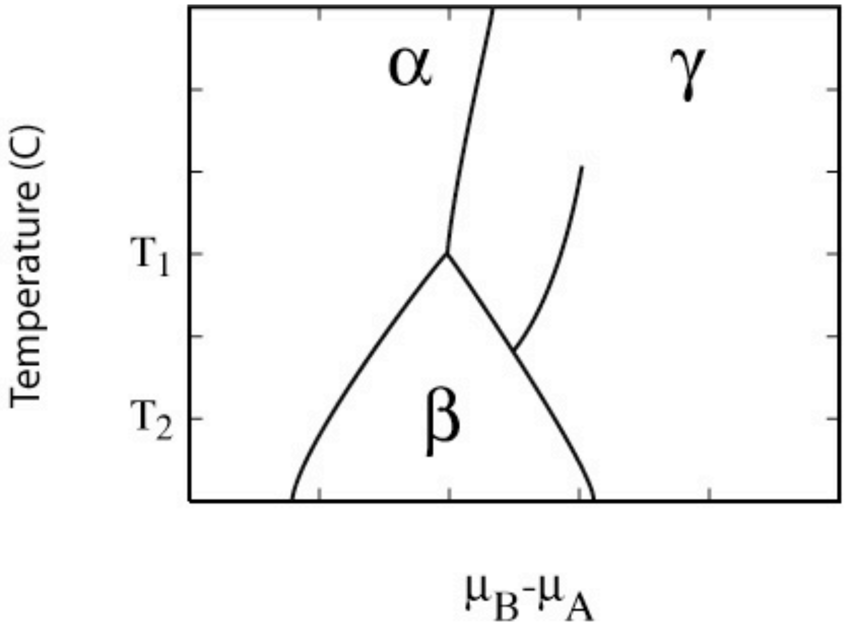
b) Consider a pipe with closed ends with wall thickness of 10 mm and inner diameter of 0.6 mm subjected to 20 MPa internal pressure and a torque of 1200 kN.m. What is the safety factor against yielding at the inner wall if the pipe is made of a steel whose yield strength is 1791 MPa?

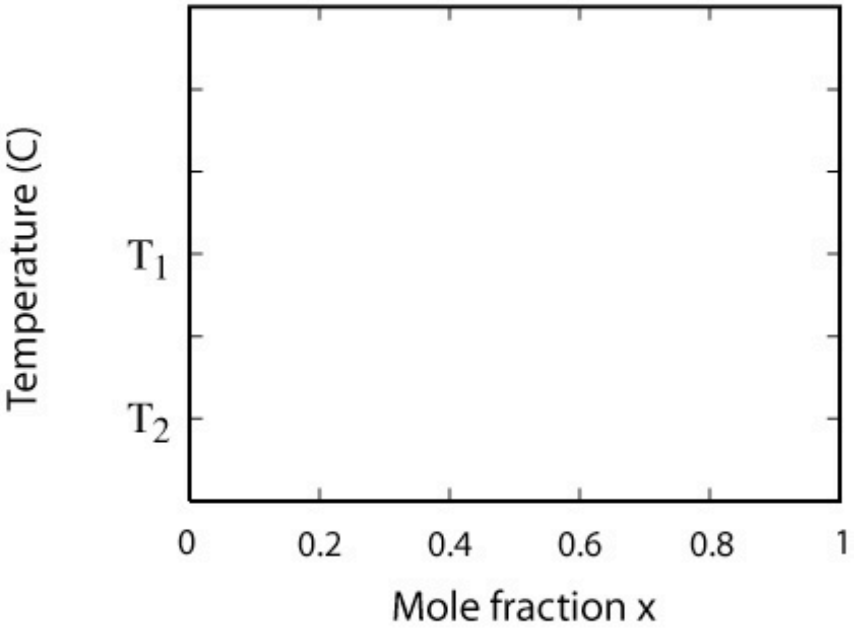
6.

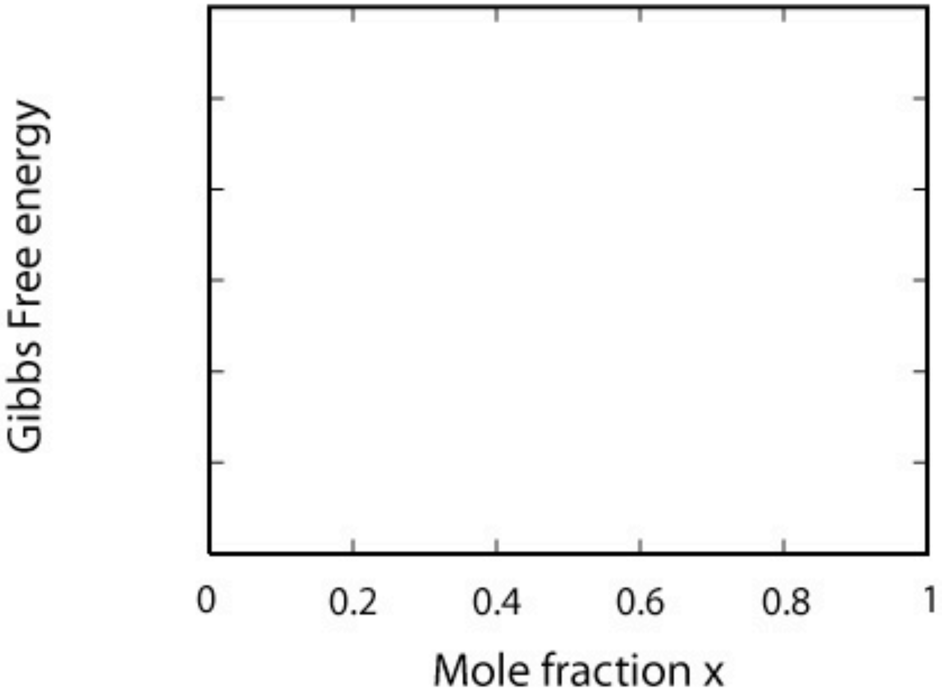
The spacing between precipitates can be important in determining the amount of strengthening produced in an alloy. Assume distribution of spherical precipitates of shear strength k_s, arranged in cubic lattice corner positions. Assume that diameter of precipitates as 15 μm and volume fraction 7%. If you now change that spacing between the precipitates to be 1/100 of the first case without changing volume fraction, dislocations are found to just cut through precipitates. Determine the strength of the alloy for the two cases by assuming that solid solution has shear strength of $k_s/3$, its shear modulus is G and dislocation Burgers vector is b.

7.

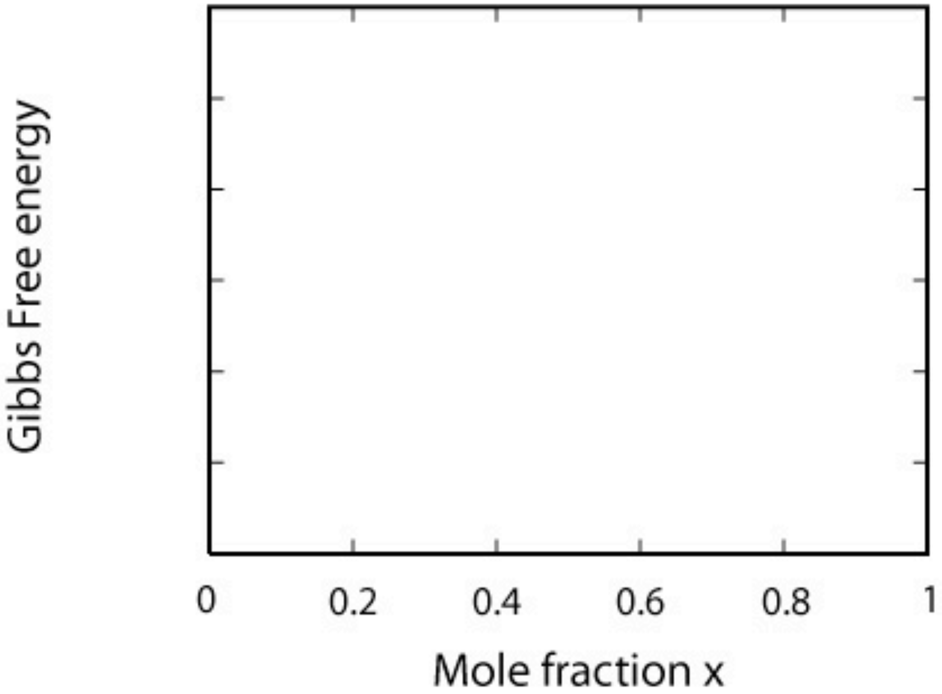
Below is a phase diagram for a binary A-B alloy expressed in terms of intensive variables (T versus μ_B-μ_A).
a) Redraw the phase diagram in terms of temperature and alloy concentration *x*.
b) Schematically draw the free energy curves at T_1.
c) Schematically draw the free energy curves at T_2.





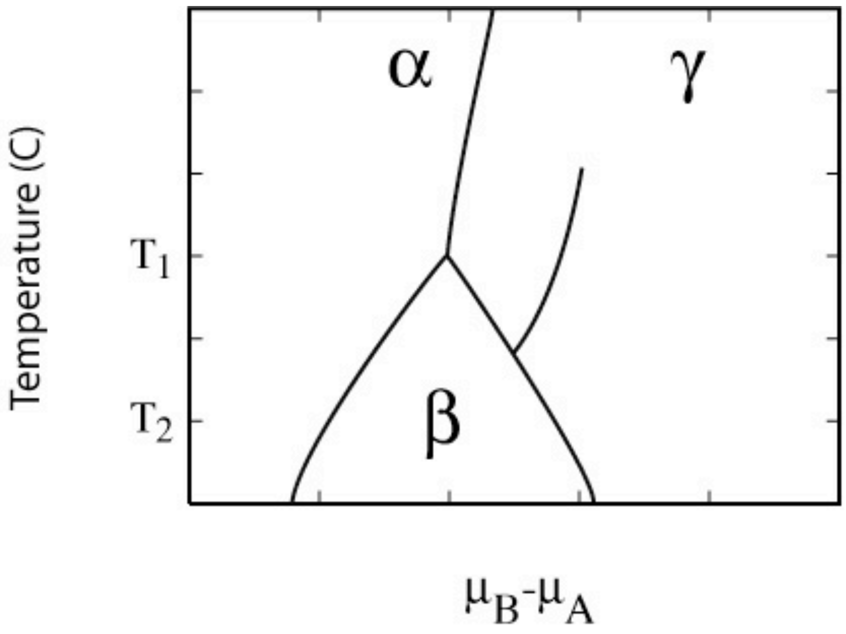

At T_1

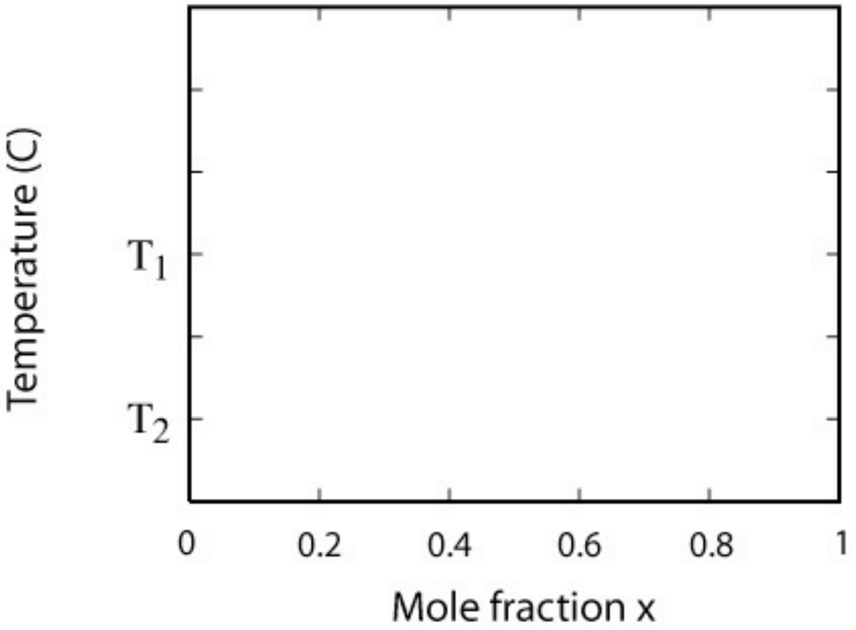
Gibbs Free energy
0
0.2
0.4
0.6
0.8
1
Mole fraction x


At T_2

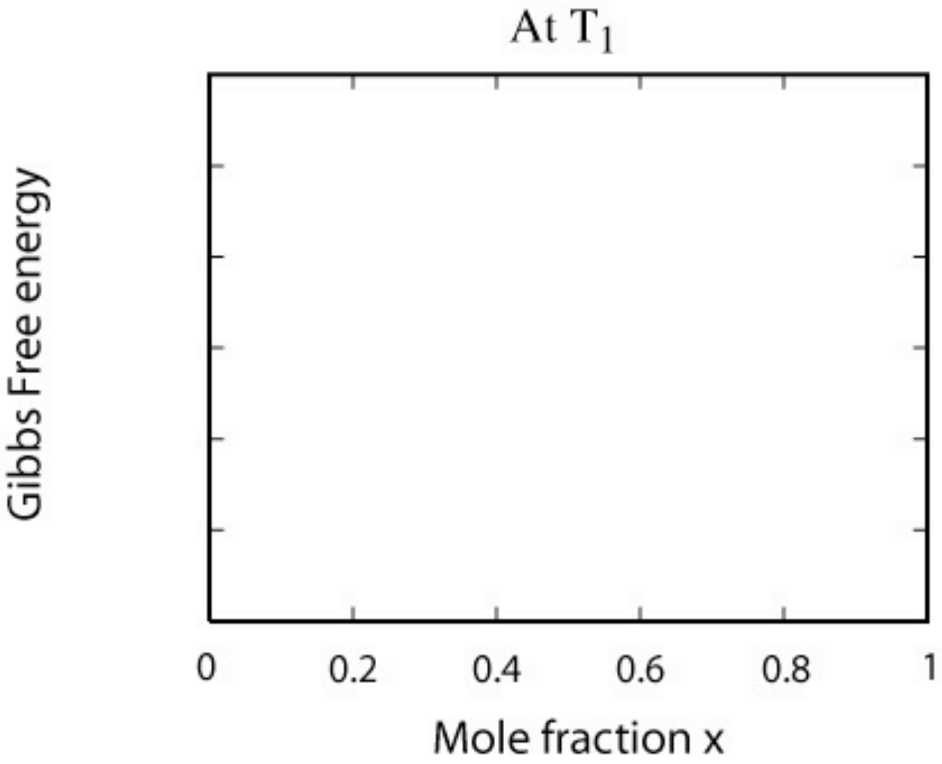
Gibbs Free energy
0
0.2
0.4
0.6
0.8
1
Mole fraction x

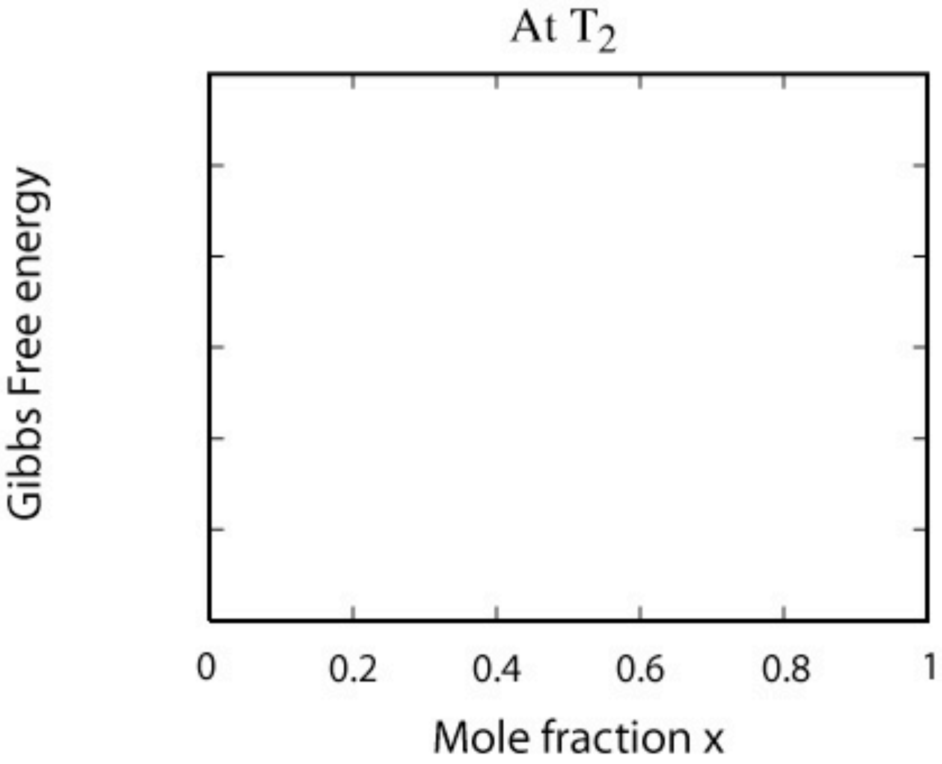
Second try if you made mistakes in the plots on the first templates:





Second try if you made mistakes in the plots on the first templates:





8.

A linear polymer is made up of M monomers. The electrons of the covalent bonds in each monomer can be in one of two states: a ground state with energy ε_o and an excited state with energy ε_1. The equilibrium length of each monomer is l_o in the ground state and l_1 in the excited state. The covalent bond within each monomer has a force constant f_o in the ground state and f_1 in the excited state (that is when the spacing between the atoms within each monomer deviates from its equilibrium value by ξ, the energy of the bond increases harmonically by $\frac{1}{2} f \cdot \xi^2$).

a) Assume that all monomers stay in their electronic ground state (i.e. $\varepsilon_1 >> \varepsilon_o$ such that the electrons of the monomers are never excited out of their ground state). Derive a closed form expression for the partition function of the linear polymer at constant temperature T and fixed polymer length M. You can assume that the ends of the polymer are at constant force F=0.

b) Now assume that the electrons of the monomers can be excited. At constant temperature T and fixed polymer length M, rederive an expression for the appropriate partition function. Again you may assume that the ends of the polymer are at constant force F=0. Make sure to derive a closed form expression by summing over all microstates.

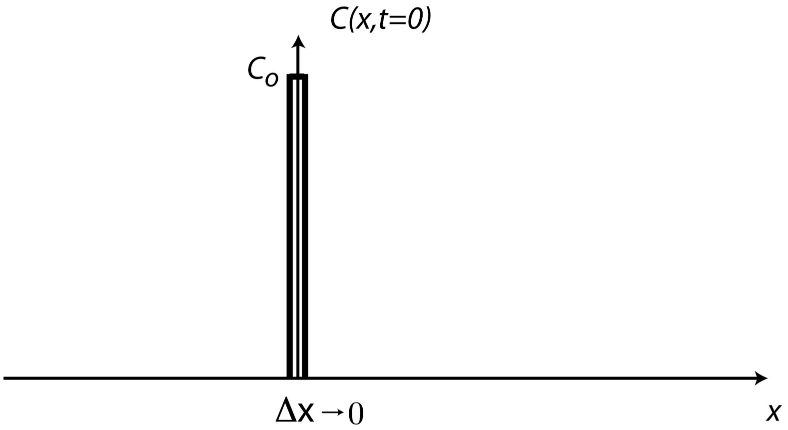
c) Write down an expression for the probability $\mathrm{P}(N)$ that N monomers are in their excited electronic state.

9.

Derive an expression for $\left(\frac{\partial T}{\partial P}\right)_U$ in terms of measurable response coefficients (e.g. C_p, β, κ etc.) and easily measurable thermodynamic state variables. (T is the temperature, P is the pressure and U is the internal energy).

10.

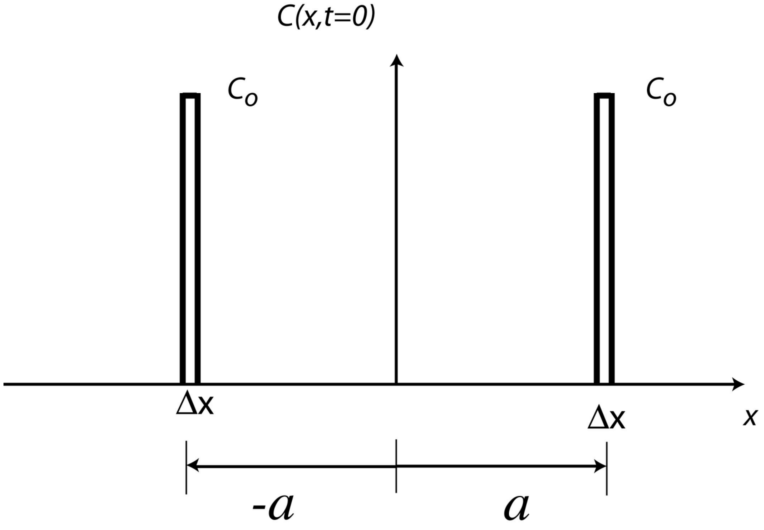
a) For the initial concentration profile (t=0) plotted below (a Dirac δ-function), write down (no need to derive it) an expression for the concentration profile $C(x,t)$. For some time t>0, make a sketch of this concentration profile.



b) Using the functional form for $C(x,t)$, derive an expression for the mean squared displacement $\langle R^2 \rangle$ of particles at time t.

c) What is the actual distance traveled, on average, by a particle at time t (i.e., counting both displacements in positive and negative x-direction). To this end, assume that particles jump once per nanosecond by a distance of 1Å.

d) Using your answer from part (a), write an expression for $C(x,t)$ at some t>0 for the initial concentration profile plotted below. Also make a careful sketch of this concentration profile at t>0.



11.

a) Derive an expression for an adsorption isotherm for a two-component gas. Assume a single layer maximum coverage, and that the adsorption energy for each component is different.

b) Consider Ar gas at 100K. Upon physisorption on solid carbon, its Gibbs free energy is lowered by 3.6 kJ/mol. Condensation of Ar, however, would release 0.8 kJ/mol less at that temperature. Assuming that multi-layer adsorption can occur, calculate the partial pressure (with respect to the saturation pressure) of Ar, at which the equivalent of two layers have been adsorbed on the carbon.

c) Calculate the number of layers that it takes in reality to accommodate 95% of this amount.

12.

Consider the geometric configuration of two phases α and β given in the diagram below (right hand side). This configuration corresponds to a situation in equilibrium at T_1 of the adjacent phase diagram. The system is cooled abruptly to T_2.

a) Superimpose the concentration profile after some time (sufficient for the effects to be visible, but still far from equilibrium). Make sure the direction of migration of the interface is obvious from your sketch.

b) Develop an expression for the velocity of migration of the interface based on the diffusivity of A in β. Assume that the change in solubility of B in α is negligible.