

NAME: _____

COURSE 3.20: THERMODYNAMICS OF MATERIALS

FINAL EXAM, Dec 18, 2000

PROBLEM 1 (10 POINTS) _____

PROBLEM 2 (15 POINTS) _____

PROBLEM 3 (12 POINTS) _____

PROBLEM 4 (12 POINTS) _____

PROBLEM 5 (12 POINTS) _____

PROBLEM 6 (15 POINTS) _____

PROBLEM 7 (12 POINTS) _____

PROBLEM 8 (12 POINTS) _____

TOTAL (100 POINTS) _____

You can either write your answer on the question sheets or use separate pages. In each case make sure your answer is clearly marked.

A neat answer is the sign of a clear mind

Question 1:

A turbine is extracting mechanical work from steam at high pressure in a steady state process. The temperature of the steam is 400°C at the inlet and its pressure is 20 atm. At the outlet the temperature is 200°C and the pressure 1.5atm. The rate of steam through the turbine is 300 moles/second. The turbine itself operates adiabatically.

- a) What is the rate of the entropy change of the turbine ?
- b) What is the entropy change of the steam per mole going through the turbine ?
- c) What is the rate of entropy change for the universe ? Only consider the process as described. Do not consider how the steam might be generated.

DATA: Heat capacity of steam can be approximated to 37 J/mol-K in this temperature range.

This Material was not covered in F2001**Question 2:**

a) What can you say about the sols, A and B, from the following information concerning the relative molar critical coagulation concentrations (CCC's)? CCC's (Relative concentrations)

Electrolyte	Sol A	Sol B
KCl	64	64
MgCl ₂	32	1
Na ₂ SO ₄	1	32

b) Draw curves that depict the potential energy of interaction $V(h)$ between two colloidal particles as a function of their separation h for the following conditions (express relevant energies in units of kT):

- (1) a stabilized sol that experiences slow coagulation; and
- (2) a sol that experiences rapid coagulation.
- (3) How do you convert a sol from condition (1) to condition (2)?

This Material was not covered in F2001

Question 3

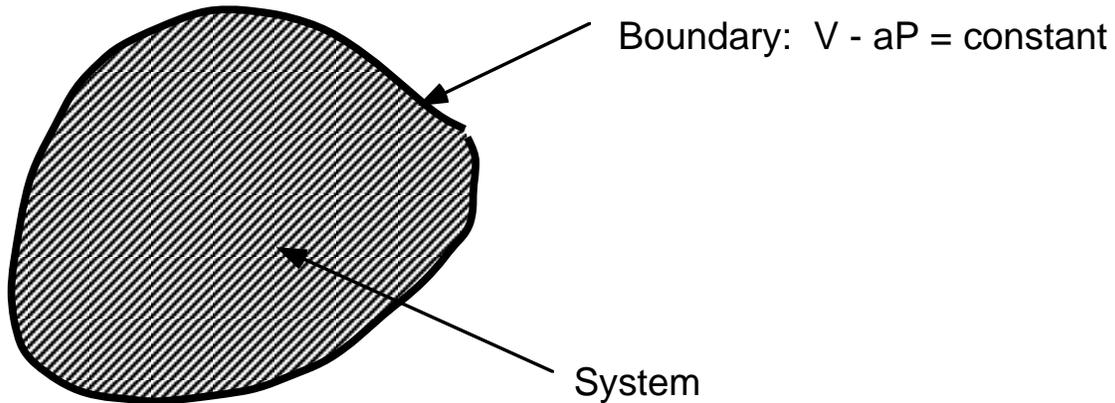
For n-octane, the surface tension is 21.8 mJ/m², and the interfacial tension on water is 50.8 mJ/m². Comment on the long-term spreading behavior of this hydrocarbon on water. (The surface tension of water is 72.8 mJ/m².)

Question 4:

Note: This is a somewhat more difficult problem

You may remember that in general, the heat capacity of a system depends on the conditions under which heat is put into the system (since δQ is path dependent). This is why for a *simple* system (that can be described with only *two state variables*) we defined a constant pressure heat capacity (C_p) and a constant volume heat capacity (C_v). This question deals with finding the effective heat capacity when a path is neither constant pressure nor constant volume.

A simple system is enclosed in an elastic balloon which expands under increased pressure exerted by the system so that $V - aP$ remains constant, and a is some parameter. Find the heat capacity under these conditions in terms of the basic properties of simple systems (C_p , α_V , β_T , a , etc.).



Question 5:

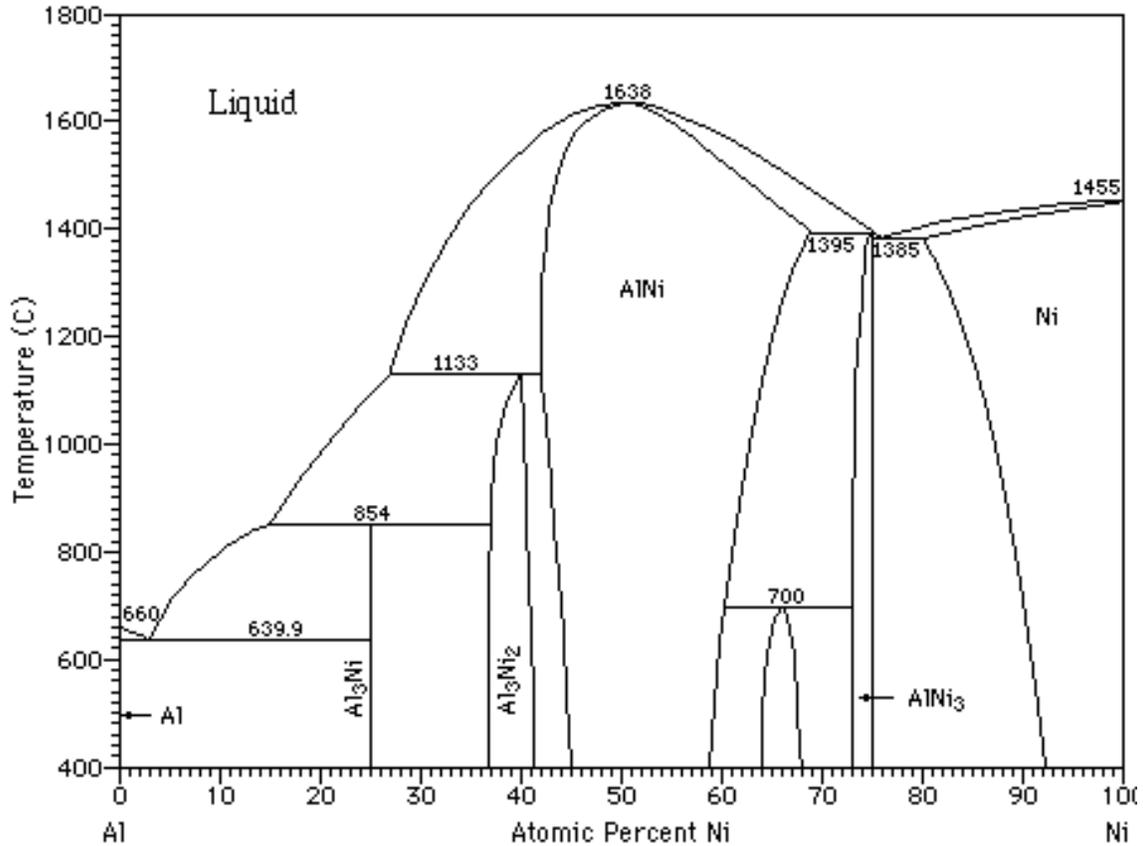
a) Sketch the heat capacity C_v as function of temperature for an elemental solid in the Einstein model. Please label the axis. Pay attention to limiting values and mark them on your graph in units of R (the gas constant).

b) Discuss clearly the *mechanism* that makes the heat capacity go to zero as the temperature goes to zero. No equations necessary.

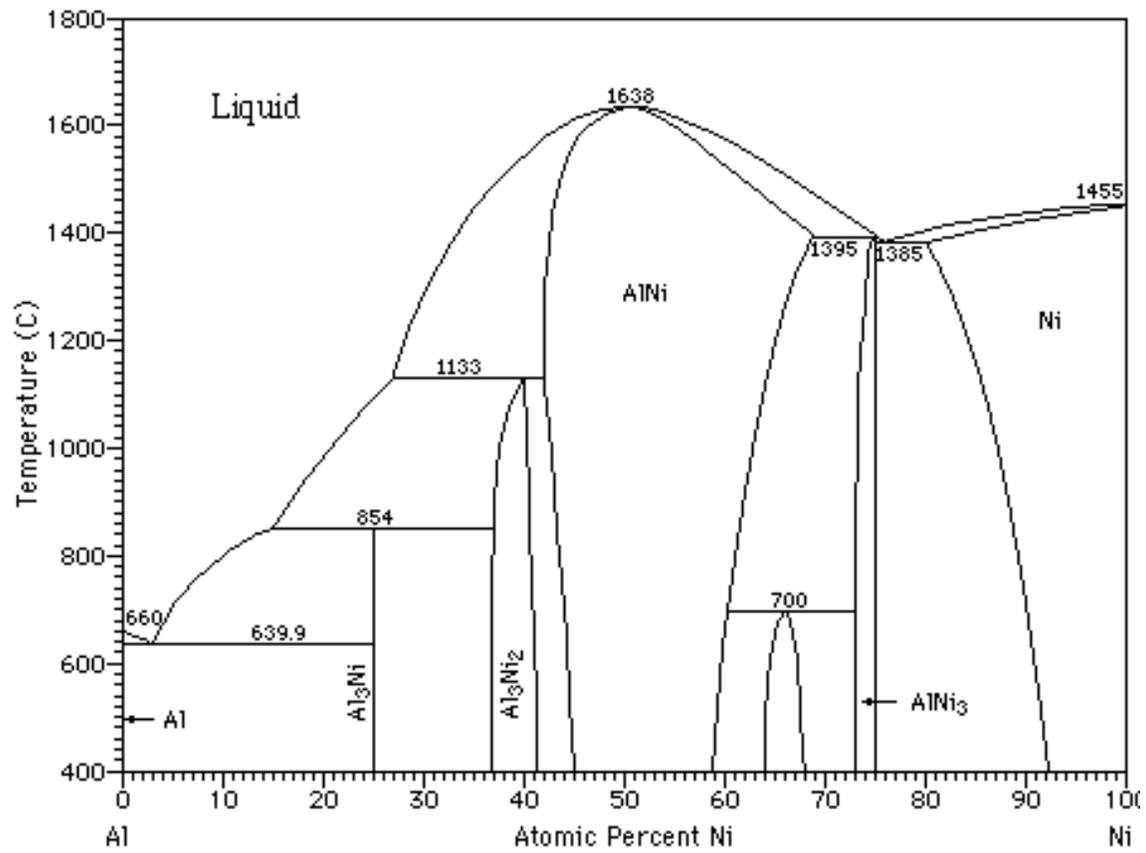
c) If I were to model the same system with a *classical* molecular dynamics simulation and plot the heat capacity from the simulation (e.g. calculated as the derivative of the energy with temperature) as a function of temperature what would it look like? Make a *plot* again marking all the limiting values. *Explain*. Think carefully of why the heat capacity goes to zero in part a).

Question 6:

Below is the Al-Ni phase diagram.



- Consider an alloy with 70 atomic percent Ni present. If this alloy is held at 1000°C, which *phases* are present and what is their *composition*? Also calculate *how much* of each phase is present.
- Describe the reaction occurring at 700°C upon cooling.
- Sketch the free energy of mixing as function of composition at 750°C for all relevant phases in the phase diagram. Pay attention to slopes, tangents, intercepts etc.
- An extra copy of the phase diagram is provided below. On this copy sketch how the phase diagram would look if the Al₃Ni₂ would be prevented from forming, but all other phases reach equilibrium with each other. Please also mark the lines that should be deleted.



Problem 7

Consider the capacitor below. It is characterized by the following extensive variables: thickness of the dielectric l , charge on the capacitor q and entropy S . The conjugate variables are force f , electrical potential ϕ , and temperature T . The characteristic function U is a function of $U(S, l, q)$.

a) In many practical cases it is easier to control T and f . Define the *Legendre transform* $B(T, f, q)$ that gives me a thermodynamic potential with natural variables T , f and q , and write its *differential*.

b) The properties of this system are defined by all the possible second derivatives of this Legendre transform. How many different properties are there? Write the matrix of second derivatives of B in terms of the following properties.

C : Heat capacity

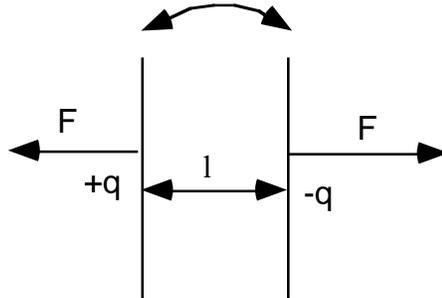
α Linear thermal expansion

Cap : capacitance (Use Cap to distinguish from heat capacity)

d : piezoelectric coefficient (measure of potential change with force)

p : pyroelectric coefficient (measure of potential change with temperature)

A : elastic compliance



Problem 8

- a) Assuming that Ga and As form an ideal solution in the liquid phase, estimate the melting temperature of the compound GaAs. The GaAs compound may be considered to be a line-compound (i.e. it allows no off-stoichiometry or disorder).
- b) The real transition temperature is 1,511K. Explain why the temperature you find is higher.

DATA:

The formation energy of GaAs (s) from solid Ga and As is:

$$\Delta G_f = -74,100 - 12.5T \text{ (in J/mole, T in Kelvin)}$$

For pure Ga:

T_m is 303 K

$$\Delta G_m = 6620 - 21.85 T \text{ (in J/mole, T in Kelvin)}$$

For pure As:

T_m is 1090 K

$$\Delta G_m = 5604 - 5.14 T \text{ (in J/mole, T in Kelvin)}$$