Homework #1

Spring 2016

Due date: February 23rd in class (hard copy print out).

ECE 6307 – Nanomaterials and Solar Energy, CHEE6320 -Introduction Nanomaterials Engineering, MTLS6320 - Nanomaterials Engineering, CHEE5320 – Introduction to Nanomaterials Engineering ECE5320 - Introduction to Nanomaterials Engineering, MECE5320- Introduction to Nanomaterials Engineering,

Student Name ____

Student ID ____

Instructions: The first page of this HW assignment has to be incorporated into your material HW. Make sure this page is signed and has your information. Students, your work (hard copy) has to be handed to the instructor at the indicated due date. Make sure your HW is typed in MS work or similar software. Handwritten submission will not be accepted. Exceptions applies to sketches that should be explanatory to your derivations or problem posting. Only independent work will be granted points. Work in the group, consulting among the students, or other type of collaboration is strictly forbidden. Student who violate this rule will be subject to the college academic honesty hearing. Problems with * marking indicate also the question that could occur on your midterm/final exam. Bonus problems are not mandatory, but could bring you extra points.

Student Signature ____

Points________________/_______35________

Problem 1. (1)

In two-tree sentences explain meaning of nanomaterials and what is important about them.

Problem 2. (1)

Give an example of nanomaterial. Explain what are the benefits of reduced scale of this material/object as compared to bulk?

Problem 3. (1)

Assume that nanoparticle has a spherical shape, derive the expression for surface to volume ratio as a function of particle radius.

Problem 4. (1) BONUS

Consider nanoparticle which has a shape of cube, octahedron, and cuboctahedron, each having the same length of an edge "a". Find out which one has the largest surface to volume ratio expressed as a function of the "a".

Problem 5. (2)

Consider zirconia nanoparticle with spherical shape and radius r=4 nm. Under careful insitu TEM investigation, these particle is found to jumps off the surface back and forth with an average amplitude of 25 cm. Find out what is the temperature T (K) in the TEM chamber, if the thermal fluctuations are responsible for this nanoparticle dynamics. ρ(zirconia)=5600 kgm^{-3}.

Problem 6. (2)

If gold nanoparticle, diameter D=5 nm is exposed to electromagnetic radiation, its temperature spikes for 17K due to an energy absorption process. The particle of unknown size exposed to the same radiation experiences temperature increase of 22 K. What is the difference in diameter of these two particles?, Assume that Cp(Au)=550 $Jkg^{-1}K^{-1}$ and ρ(Au)=20 $kgcm^{-3}$.

Problem 7. (2) BONUS

Considering two gold particles with diameters of 10 μm and 5 nm. They have a monolayer of Ag deposited on their surfaces. They are heated to a temperature of 500 K until the complete homogenization is achieved in each of them. The 5 nm nanoparticle is homogenized for 10,000 X shorter time than 10μm particle. Find out what is the activation energy for the diffusion of silver in gold.

Problem 8. (1)

List one example where nanoparticle material is used to fabricate device. Explain what properties at nanoscale material are beneficial for given device performance. (Do not write more than 4 sentences).

Problem 9. (3)

Assume that the thickness of near surface region is 1 nm. Plot the volume fraction of spherical nanoparticle material affected by the surface as a function of nanoparticle diameter. Do the same for cubic and tetragonal nanoparticle.

*Problem 10. (2)

In step by step sequence, derive the expression for surface energy of nanoparticle ($U_{surface}$ [$Jmol^{-1}$]), assuming γ as a surface energy [Jm^{-2}], M as molar mass of material [$kgmol^{-1}$], ρ as density of material [kgm^{-3}]. Do this for spherical and cubic shape nanoparticles.

Problem 11 (2)

Assume 1 mol of Au in a solid chunk and as an assembly of nanoparticles with diameter D=20 nm. Which form of material has a larger total energy and how many times larger. Assume cubic Au nanoparticles.

Problem 12 (3) BONUS

Assuming a simple cubic structure of a material, show which of the closed packed planes ((111), (110) or (100)) has the lowest surface energy. Show your derivations, drawings, and assumptions. (hint; Use basic definition of surface energy as # of broken bonds per unit area).

Problem 14 (2) BONUS

Assuming the thermodynamic definition of surface stress as:

$$f = \gamma + \frac{d\gamma}{d\epsilon}$$

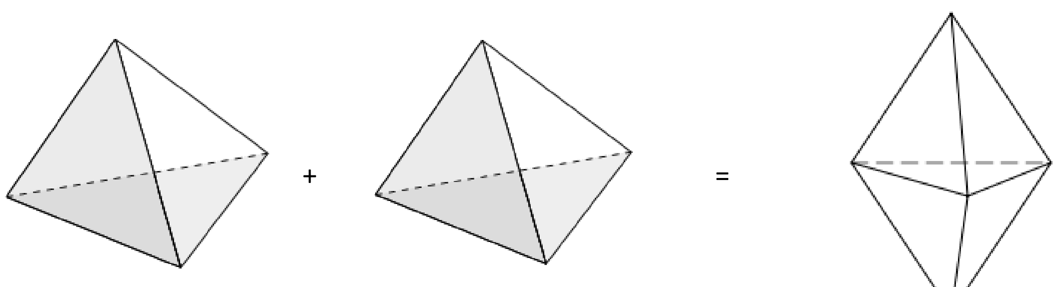
and interpreting the surface energy as #of broken bonds per surface area of a simple cubic crystal structure, show what is expected value of surface stress for the value of surface energy of 1 Jm^{-2}. The elastic limit of solid is assumed to be ±10%.

*Problem 15(2)

Combining the basic definition of Gibbs free energy [J]:
G=U + PV – TS
And 1st and 2nd law of thermodynamics in a step by step process derive the expression showing that
dG=-SdT+Vdp
In a similar procedure, show that this expression is valid for Helmholtz free energy:
dF=-SdT-pdV

Problem 16 (1)

During the fusion of two identical tetragonal nanoparticles a new one is formed with tetragonal bi-pyramidal shape. The fusion process occurs at T=450K. Cp=500 $Jkg^{-1}K^{-1}$, r=20 gcm^{-3}.



Assuming the surface energy value of 1 Jm-2, and length of the nanparticle edge to be 5 nm, find out what is the temperature of fused particle immediately after the fusion process.

Problem 17. (2) BONUS

In the previous problem, add in the energy balance the change in the strain energy of the particles during a fusion process. Assuming new energy balance, calculate the temperature of a fused nanoparticle. Kv=300 MPa. Explain in detail all approximation used in your calculations.

*Problem 18. (2)

Starting from Clausius-Clapeyron eq. and expressing the pressure in two different equilibrium states at different temperature as a function of the local curvature of the material (all equations are in your notes and book), derive the expression which can be used to model melting temperature of nanoparticles as a function of their size. Show every step.

*Problem 19. (2)

Starting from Hooks law for nanoparticle, and assuming the arguments for pressure on the nanoparticle as a function of its size, derive in a step by step process an expression for absolute contraction of the lattice constant Δa as a function of the nanoparticle diameter.

$\Delta a = f(D_{nanoparaticle})$

Problem 20. (3) Bonus

Assume the fusion of two nanoparticles of diameter D results in temperature increase, ΔT. At the same time, considering result from problem 18, we know that the melting temperature of Au nanoparticles is a function of their size. Derive the expression for the size of fusing Au nanoparticles at which the melting temperature of a new –fused nanoparticle will be exceeded.

Do the same but consider that only 20% of the fused nanoparticles might be melted.