Massachusetts Institute of Technology

Mathematical Methods
for Materials Scientists and Engineers

3.016 Fall 2010

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Problem Set 7: **Out: 25 Oct.** and **Due: 11 Nov.**

Individual assigments should be a combination of your hand-worked solutions and other printed material—they should be placed in the mailbox outside Prof. Carter's door. Email group assignments to 3016-psets(the symbol at)pruffle.mit.edu

For the individual problems indicated as "Handworked", you should work your solutions by hand and show your work. Print the results of software-worked solutions, and staple them to your hand-worked assignments before turning them in.

The following are this week's randomly assigned homework groups. The first member of the group is the "Jomework Jefe" who will be in charge of setting up work meetings and have responsibility for turning in the group's homework notebook. If some some reason, the first member in the list is incapacitated, recalcitrant, or otherwise unavailable, then the second member should take that position. *Attention slackers:* The Jefe should include a line at the top of your notebook listing the group members that participated in the notebook's production; only those listed will receive credit. Group names are boldfaced text.

Beanie: *ronrose, llena, pmelo, hekopp*

Beret: *andy_c, sojung, elomeli, aliciac*

Boater: *viviand, chandrak, ezuniga, bwee*

Bowler: *yhelen, dimitri_, vtrevino, tsarathi*

Fez: *ssluo, eperry4, jchenlia, m_gibson*

Homberg: *ckopp, tsmickel, jrm90, aypark*

Kepi: *ernmart, msee, spuranam, nsinatra*

Montera: *changey, mcjasso, jschein, amelanie*

Individual (Handworked) Exercise I7-1

(You may wish to use a combination of software and "pencil-and-paper" on this problem. For you pencil and paper work, enter text equations, or drawings that illustrate your primary results and reasoning.)

An important concept throughout materials science is that of "coarsening" of a two-phase microstructure (e.g., particles of one phase in a matrix of an another phase.). Coarsening is a process that changes the microstructural length scale of a system and—in the case of particulate two-phase microstructures—results in the disappeance of some particles. "Ostwald ripening" is a a well-known example of coarsening.

Coarsening processes are driven by reductions in the total interfacial energy. This problem will illustrate the driving forces and a simple model for the coarsening rate. It is remarkable how illustrative this simple problem is for many materials science applications.

The total surface energy of an interface is

$$F_{\text{interface}} = \int_{\substack{\text{all} \\ \text{interfaces}}} \left(\gamma_i \hat{n} \cdot d\vec{A} \right) = \int_{\substack{\text{all} \\ \text{interfaces}}} (\gamma_i dA) =$$

where the integration is taken over all of the interfacial areas, and γ_i is the surface energy per unit area (sometimes called *the surface tension* or *superficial/interfacial free energy density*) If γ_i does not depend on position or is independent of the interface orientation (i.e., it is isotropic) then,

$$F_{\text{interface}} = \gamma_i \int_{\substack{\text{all} \\ \text{interfaces}}} dA = \gamma_i A_{\text{interfaces}}$$

Here is an example of a system that can change its interfacial area: either volume can be exchanged between the two bubbles, or volume can be added to one of the bubbles indendently.
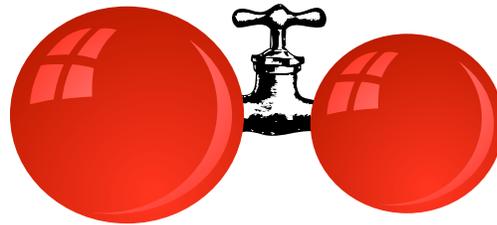
1. Consider the addition of volume to single bubble as in the left-hand figure. Find an expression for the pressure difference between the inside and the outside of a single bubble with volume $V = 4\pi R^3/3$. To do this, suppose that the system is at constant temperature, and that the Helmholtz free energy is $dF = -SdT - PdV$. Supposing that all of the Helmholtz free energy change is accounted for by the interfacial energy, find a relationship between the bubble's external and internal pressure, γ_i, and the radius of the bubble R. Do this by equating the reversible work with the change in total Helmholtz free energy.

2. Suppose the valve between the two bubbles in the right-hand figure is closed. Find an expression for the pressure across the valve.

3. Suppose that the valve is opened slightly and that the the volumetric rate of flow is proportionaly to the pressure difference. Construct a model for the evolution of the volumes of the two bubbles starting with initial volumes V_{right} and $V_{\text{total}} - V_{\text{right}}$. Describe an illustrate the model's behavior. (Treat the gas as incompressible, i.e., V_{total} is constant.)

4. Suppose you did a physical experiment. How would the system behave if you made the intial states as $V_{\text{right}} = V_{\text{total}}/2$? Think carefully.

Individual Exercise I7-2

The magnetic vector potential of a magnetic dipole located at the origin is given by

$$\vec{A}_{\text{dpl}} = \text{constant} \frac{\vec{\mu} \times \vec{r}}{|\vec{r}|^2}$$

The magnetic field is related to the magnetic vector potential by $\vec{B} = \nabla \times \vec{A}$.

1. Find the magnetic field of a dipole.

2. Show that the magnetic field of the dipole satisifies Maxwell's equation for the magentostatic condition: $\nabla \cdot \vec{B}_{\text{dpl}} = 0$.

3. Visulize the magnitude of the magnetic vector potential for a dipole.

4. The torque between two magentic dipoles is $\mu \times \vec{B}_{\text{dpl}}$, calculate energy difference between two parallel (i.e., ↑↑) and antiparallel dipoles (i.e, ↑↓) for dipoles that are fixed in space. Visulize this energy difference.

Individual Exercise I7-3

Here is some code to visualize an FCC crystal:

```
latticeVectors = {{8, 0, 0}, {0, 8, 0}, {0, 0, 8}};
motifVector = {4, 4, 0};
corners =
  Flatten[
   Table[
    i latticeVectors[[1]] +
      j latticeVectors[[2]] +
     k latticeVectors[[3]],
    {i, -1.5, 2.5, 0.5},
    {j, -1.5, 2.5, 0.5},
    {k, -1.5, 2.5, 0.5}], 2];

faces = Table[corners[[i]] + motifVector, {i, 1, Length[corners]}];

Graphics3D[
 {
```

```
  {Blue, GraphicsComplex[corners,
    Table[Sphere[i], {i, 1, Length[corners]}]]},
  {Blue, GraphicsComplex[faces,
    Table[Sphere[i], {i, 1, Length[faces]}]]}
  }
]
```

1. Modify this code to draw the Rocksalt crystal structure.

2. Previously, you used the displacement field of a dislocation to calculate its stress field. Use this displacement field and apply it to each of the atom positions to visualize the dislocation displacement field in an FCC crystal.

Group Exercise G7-1

Interstitial defects will diffuse in response to a dislocation. Because interstitials tend to make the surrounding lattice expand, they cause a local *expansion*. These interstitials tend to diffuse towards regions of net tension (i.e., *negative hydrostatic pressure*).

This problem will explore a "Monte Carlo" method to simulate this diffusion for interstitials in the vicinity of an edge dislocation. In this simulation, the effect of temperature on the flow of interstitials will be simulated with a Metropolis algorithm (c.f., Problem G3-3 from 3.016 2008). The interstitial energy is the local pressure multiplied by the "extra volume" associated with the interstitial, $P(\vec{x})\Delta V$. Pick two or three different temperatures that illustrate the effect of temperature on the evolution on the interstitials.