ENGG 201

What is Going On with Solids?
(A Brief Outline of What is Important in Ch 3 and 9)

Chapter 3 – Notions About The Nature of Matter

Main Concepts:

1. Lennard-Jones Potential Energy Functions (Section 3.7)
    a. How do the FORCE and POTENTIAL ENERGY between molecules change with DISTANCE?
2. Bravais Lattice Structures in Solids (Section 3.8)
    a. How do molecules in SOLIDS arrange themselves and how does the STRUCTURE influence the DENSITY?

Things to Remember:

Lennard Jones

1. LJ potential functions can be used for gases, liquid or solids (mostly for solids).
2. The potential energy is the integral of the force over a distance (from infinity to r).

$$\Phi(r) = \int_{\infty}^{r} F(r)dr$$

3. The Force is the derivative of the Potential Energy $F(r) = \frac{d\Phi(r)}{dr}$
4. The LJ potential energy function $\Phi(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$ is a SPECIFIC function for the potential, but there are others – make sure you understand how to go between F and Φ and back again.
5. Simplify expressions BEFORE subbing numbers in. [For example if you have a $(\sigma/r_o)^{12}$ term, and r_o=1.122σ, make your expression $(1\sigma/1.122\sigma)^{12}=(1/1.122)^{12}$]
6. To find the minimum of anything, take the derivative and make it equal to zero - Minimum potential energy ($\Phi_{min}= -\varepsilon$) occurs when the force (F) is zero.

$$F(r) = \frac{d\Phi(r)}{dr} = 0$$

7. Attractive FORCE is + and Repulsive FORCE is -.
8. Attractive ENERGY is – and Repulsive ENERGY is +.

Lattice Structures / Density

9. In most cases, the atomic diameter (d) can be taken as equal to the collision diameter (σ).
10. The atomic diameter (d) is not always equal to the length of one side of the unit cell (Only true for cubic, NOT FCC or BCC).
11. Make sure you know what the cubic, FCC and BCC arrangements LOOK like, as well as the formulas for the density of each.
12. Density = mass / volume is for a unit cell. The mass is the mass of the number of atoms in the unit cell (not always 1) as a function of the molar mass, and the volume is the size of the unit cell as a function of the molecular diameter.

<u>Examples of Typical Problems:</u>

Lennard Jones

1. Given an equation for Φ, derive an equation for F.
2. Given an equation for F, derive an equation for Φ.
3. Calculate the separation distance (r) for a certain F or Φ (including at minimum Φ).
4. Calculate the F or Φ for a given r.
5. Calculate σ for a given F or Φ and r.

Lattice Structures / Density

6. Calculate ρ for a given M and d (or length of side of unit cell) and structure.
7. Calculate M for a given ρ and d (or length of side of unit cell) and structure.
8. Calculate d (or length of side of unit cell) for a given M and ρ and structure.
9. Calculate structure for a given M and d (or length of side of unit cell) and ρ.
10. More … (See old finals).

Chapter 9 – The Structure and Transport Properties of Solids

Main Concepts:

Thermal Properties and Heat Conduction (Section 9.2)

1. Heat Capacity
   a. How are HEAT and TEMPERATURE related?
2. Thermal Expansion
   a. How is a change in TEMPERATURE related to a change in SHAPE?
3. Thermal Conductivity (*)
   a. How is the RATE OF HEAT TRANSFER related to the TEMPERATURE difference, DISTANCE the heat has to travel, and the THERMAL CONDUCTIVITY of the material?

Things to Remember:

Heat Capacity

1. The amount of heat (Q) lost (-) or gained (+) can be calculated from $Q=mC\Delta T$.
2. Cp of solids can be estimated as 3R (only if not given).

Thermal Expansion

3. The change in length for a solid as a result of a temp change can be calculated using $\alpha_L = \frac{1}{L}\frac{dL}{dT}$, where α_L is the coefficient of linear thermal expansion.
4. In the above equation, *dL/L* is the fractional change in length. Use numbers, not percents (i.e. if the fractional change in length is 3%, use 0.03 as dL/L).
5. A positive *dT* (temp increase) gives a positive *dL* (increase in length).

Thermal Conductivity

6. **Always draw a diagram** and label a) Temperatures (T_1, T_2, etc), b) Names and number of each layer (Layer 1 = insulation, etc.), c) Thermal conductivity of each layer (k_1=0.05 W/mK, etc.), d) dimensions such as thickness of each layer and radius, e) Direction of heat flow.
7. Fourier's Law for a simple wall $Q = -\kappa A\frac{dT}{dx} = -\kappa A\frac{\Delta T}{\Delta x}$, where Q is the RATE of heat conduction, and heat always flows from high to low temperature

8. For a composite wall, the overall resistance is the sum of the resistance offered by each layer $Q = \dfrac{-A\,\Delta T}{\left[\dfrac{\Delta x_1}{\kappa_1} + \dfrac{\Delta x_2}{\kappa_2} + \dfrac{\Delta x_3}{\kappa_3} + \ldots\right]}$
9. Fourier's Law for a simple cylinder $Q = \dfrac{-2\pi\kappa L\,\Delta T}{\ln\left(\dfrac{r_2}{r_1}\right)}$
10. For a composite cylinder, the overall resistance is the sum of the resistance offered by each layer $Q = \dfrac{-2\pi L\Delta T}{\dfrac{\ln(r_2/r_1)}{\kappa_1} + \dfrac{\ln(r_3/r_2)}{\kappa_2} + \dfrac{\ln(r_4/r_3)}{\kappa_3} + \ldots\ldots.}$
11. **FOR ALL CASES, calculate the ΔT by going in the OPPOSITE direction to the Q that you have drawn (for example if Q goes from point 1 to point 3, then $\Delta T=T_3-T_1$).**
12. **In composite (more than one layer) walls / pipes / spheres, the overall rate of heat transfer (Q) is the same as the heat transferred through each layer ($Q_1=Q_2=Q_3=\ldots=Q$).**
13. This means that Fourier's law can be written for a) Each individual layer, b) All the layers together, or c) Any number of adjacent layers. (If you have three layers – 1,2,3 – then you can write $Q_{123}=Q_1=Q_2=Q_3=Q_{12}=Q_{23}$ where Q_x is the heat transferred through layer x).

<u>Examples of Typical Problems:</u>

1. Given the fractional change in L, calculate the temp change (and vice versa).
2. Given a pipe / wall (uninsulated), calculate Q for a given inside and outside temp.
   a. Then add insulation, and calculate the new Q, or the temp at the interface between the insulation and the pipe.
   b. Or, calculate the minimum thickness of insulation to give a certain Q.
3. Given a pipe / wall (uninsulated), calculate one T for a given Q and given other T.
4. Given a room/building, calculate the heat lost/gained through one/all walls. Some walls may be insulted, some may not.
5. More … (See old finals).