

3.052 Nanomechanics of Materials and Biomaterials : Spring 2007 Assignment #3

Due Date : Thursday 03.15.07

You are encouraged to use additional resources (e.g. journal papers, internet, etc.) but please cite them (points will be deducted for not doing so). You will need to research additional sources to answer some questions.

1. Heparin Biosensors Podcast: Milovic, *et al.*, "Monitoring of heparin and its low-molecular-weight analogs by silicon field effect." 13374–13379, *PNAS*, **2006**103 (36)

- Research the primary sequence of a protamine and of the chemistry of the sensor surface and based on this information explain in detail all of the possible nonspecific interactions involved in the physisorption process used for sample preparation.
- Physisorption of biomacromolecules to surfaces can be highly variable and uncontrolled; name 5 important physical properties of the coating to consider.
- On page 13378, the text says "AT-III was covalently attached to the sensor surface by..." Some scientists could disagree with this point, why?
- Why does Jon Behr say that current clinical tests for heparin levels measure heparin activity, not actual concentration? Why are current tests for heparin levels not appropriate for clinical use? How is a clinical measure of concentration a major advantage in the case of heparin?

2. Theoretical Modeling of the Mechanics of Single Cells. In Section 3.1 of Dao, *et al.* **2003** 51 *J. Mech. Phys. Solids* 2259-2280 (posted under "Supplementary Resources" on Stellar) an equation is presented for the membrane shear modulus, μ , which is not constant but is dependent upon the degree of stretch.

- Starting from the neo-Hookean strain energy potential function (equation (2), derived in recitation on 03.02.07), present the full derivation of equation (5). Show all steps in between equations (2)-(4). Be sure to justify all assumptions and equations used, and define all symbols used. Include an explicit derivation for the constant volume constraint, $\lambda_1\lambda_2\lambda_3=1$. Note that the symbol T is the membrane "stress" which is equal to the Force per unit length in units of N/m.
- Recreate Figures 3a and 3b with the horizontal axis covering up to a maximum principal stretch of $\lambda_1 = 3$.
- In Lecture, we discussed a secondary strain hardening term added to the neo-Hookean strain energy potential function. Explain one interpretation of the physical origin of this term.

N.B.: There is a typo in equation (3) and it should read :

$$T_1 = h\lambda_1 \frac{\partial U}{\partial \lambda_1} = G_0 h_0 (\lambda_1^{1.5} - \lambda_1^{-1.5}).$$

There is also a mistake in equation (5); it should read :

$$\mu(\lambda_1) = \frac{1}{2} \frac{\partial T_s}{\partial \gamma_s} = \frac{3G_0 h_0 (\lambda_1^{0.5} - \lambda_1^{-2.5})}{2(2\lambda_1 + \lambda_1^{-2})}$$

3. Intermolecular Potentials, Water, and H-Bonding.

- Consider the following contributing interactions between two water molecules; dispersion interactions, orientation polarization of freely rotating dipoles, and induced polarization (freely rotating dipole-induced dipole) which are collectively known as the van der Waals

interaction, $w(r)_{VDW}$ (do not consider H-bonding specifically yet). Plot $w(r)_{VDW}$ quantitatively in units of w ($k_B T$) and r (nm). Include a short range Coulombic repulsion term; $w(r)_{repulsive} = B/r^{12}$ with $B = 10^{-134} \text{ Jm}^{12}$.

- b. Compare the strength and equilibrium bond length of this van der Waals interaction estimation (part a) to a typical H-bond.
- c. Another model for the interaction between two water molecules is a Lennard-Jones potential plus 16 Coulombic terms. Explain the reasoning behind such a model. What would the latter terms correspond to physically?
- d. Estimate the van der Waals force of a water molecule (using the potential of part a) approaching a layer of water on a surface at a separation distance of 3 nm.
- e. The "range" of an interaction is an ambiguous concept. Why? Propose a reasonable mathematical definition for the range of an interaction.
- f. Polymethylene oxide $[-\text{CH}_2-\text{O}-]_n$ is hydrophobic but polyethylene oxide $[-\text{CH}_2-\text{CH}_2-\text{O}-]_n$ is hydrophilic. Explain why.

+ 5 extra credit for posting a message on the podcast message board.

Pset #3 : Q #2 Cell Membrane Stresses

