3.052 Nanomechanics of Materials and Biomaterials : Spring 2007 Assignment #4

Due Date : Thursday 04.24.07

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. Everything must be answered in your own words; also, do not copy phrases or sentences from the paper or podcast.

+ 5 extra credit for posting a message on one of the podcast message boards.

1. van der Waals Forces at Work : Gecko Feet Adhesion. Tian, *et al.* PNAS **2006** 99: 12252-12256.

a. Equation [16] gives an alternative geometry for calculating the van der Waals adhesion force. Define the assumed geometry and all constants according to the schematic in Figure 1i, and then use equation [16] to recreate the plot shown in Figure 4.

b. How do Figures 5 and 6 explain the roll-in, roll-out mechanism for gecko walking?

c. From the Discovery Channel movie on Professor Autumn Kellar:

i. Explain what was meant by "the gecko hairs become one with the wall."

ii. Explain what was meant by "the gecko is the Bermuda triangle of biology."

iii. Name a number of potential applications for the fundamentals behind gecko feet adhesion.

iv. What is the "Mecko Gecko"?

 $v. \ \mbox{Name 3}$ other types of biological adhesion mechanisms and the animals that use them.

2. Boundary Lubrication Podcast, Hydration Forces: Briscoe, *et al.*, "Boundary Lubrication Under Water," *Nature* 444, 9 November **2006**, 191-194.

a. Research 3 different definitions of "boundary lubrication" and 3 different technological applications where boundary lubrication is relevant (cite all sources). Professor Klein proposes that ions can behave as "molecular ball bearings" in boundary lubrication. Explain this analogy.

b. Professor Klein mentioned that "one can not take pictures with the SFA" (like the AFM can). In a few sentences, explain why not.

c. Professor Klein states that "experiments are meaningless without controls" and refers us to Figure 1 which is a control experiment. Explain in <0.5 pages how these data verify the accuracy of their experimental setup.

d. The bare mica data from Figure 1 has been digitized and is posted in an Excel file. Given the theoretical parameters provided in the Figure caption, estimate a quantitative value of the Hamaker constant in units of zJ using two separate DLVO theoretical predictions (using a linearized Poisson-Boltzmann Formulation); 1) constant surface charge and 2) constant surface potential. Include in your solutions a single plot showing the two theoretical fits compared to the experimental dataset in units of Force (mN/m) versus Distance (nm). Make sure to work out all units correctly (points will be deducted for not doing so).

e. The boundary lubrication mechanism presented in the current paper differs slightly from that proposed in Klein's previous paper on fluidity of bound hydrated ionic layers (Raviv, et al. 1540 297 **2002** *Science*). Explain how.

3. The Electrostatic Double Layer : Cartilage Podcast: Dean, et al. J. Biomech. 2006 39,14 2555.

a. For Figure 6a and b, why isn't the constant compliance regime set to D=0? Explain how this nonzero distance of the constant compliance regime is determined experimentally in <0.5 pages.

b. For Figures 6a and b calculate the distance at which repulsion due to conformational entropy begins for each salt concentration and summarize these values in a table. Compare the values obtained in the table for Figures 6a and 6b and explain any differences.

c. Given the chemical structure and dimensions of aggrecan and GAG and the aggrecan molecular surface packing density reported in the paper, estimate the areal surface charge per unit area (C/m^2) due to the GAGs at pH 5.6 (the pH at which the nanomechanical experiments were carried out).

d. Given the known amino acid sequence of the protein core backbone and the aggrecan molecular surface packing density reported in the paper, estimate the areal surface charge per unit area (C/m^2) due to the core protein at pH 5.6 (the pH at which the nanomechanical experiments were carried out). You may want to prepare a Matlab script to assist in the calculation. What is the percentage contribution to the total areal areal surface charge per unit area.

e. Based on your answers to parts c. and d., can the linearized Poisson-Boltzmann Debye-Huckel formulation be employed to predict the EDL force? Why or why not? MTTLLWVFVTLRVITAAVTVETSDHDNSLSVSIPQPSPLRVLLGTSLTIPCYFIDPMHPVTTAPSTAPLAP RIKWSRVSKEKEVVLLVATEGRVRVNSAYQDKVSLPNYPAIPSDATLEVQSLRSNDSGVYRCEVMHGIEDS EATLEVVVKGIVFHYRAISTRYTLDFDRAQRACLQNSAIIATPEQLQAAYEDGFHQCDAGWLADQTVRYPI HTPREGCYGDKDEFPGVRTYGIRDTNETYDVYCFAEEMEGEVFYATSPEKFTFQEAANECRRLGARLATTG HVYLAWQAGMDMCSAGWLADRSVRYPISKARPNCGGNLLGVRTVYVHANQTGYPDPSSRYDAICYTGEDFV DIPENFFGVGGEEDITVQTVTWPDMELPLPRNITEGEARGSVILTVKPIFEVSPSPLEPEEPFTFAPEIGA TAFAEVENETGEATRPWGFPTPGLGPATAFTSEDLVVQVTAVPGQPHLPGGVVFHYRPGPTRYSLTFEEAQ QACPGTGAVIASPEQLQAAYEAGYEQCDAGWLRDQTVRYPIVSPRTPCVGDKDSSPGVRTYGVRPSTETYD VYCFVDRLEGEVFFATRLEQFTFQEALEFCESHNATATTGQLYAAWSRGLDKCYAGWLADGSLRYPIVTPR PACGGDKPGVRTVYLYPNQTGLPDPLSRHHAFCFRGISAVPSPGEEEGGTPTSPSGVEEWIVTQVVPGVAA VPVEEETTAVPSGETTAILEFTTEPENQTEWEPAYTPVGTSPLPGILPTWPPTGAETEESTEGPSATEVPS ASEEPSPSEVPFPSEEPSPSEEPFPSVRPFPSVELFPSEEPFPSKEPSPSEEPSASEEPYTPSPPEPSWTE LPSSGEESGAPDVSGDFTGSGDVSGHLD

CS DOMAINS:

FSGQLSGDRASGLPSGDLDSSGLTSTVGSGLTVESGLPSGDEERIEWPSTPTVGELPSGAEILEGSASGVG DLSGLPSGEVLETSASGVGDLSGLPSGEVLETTAPGVEDISGLPSGEVLETTAPGVEDISGLPSGEVLETT APGVEDISGLPSGEVLETTAPGVEDISGLPSGEVLETTAPGVEDISGLPSGEVLETAAPGVEDISGLPSGE VLETAAPGVEDISGLPSGEVLETAAPGVEDISGLPSGEVLETAAPGVEDISGLPSGEVLETAAPGVEDISG LPSGEVLETAAPGVEDISGLPSGEVLETAAPGVEDISGLPSGEVLETAAPGVEDISGLPSGEVLETAAPGVE EDISGLPSGEVLETAAPGVEDISGLPSGEVLETAAPGVEDISGLPSGEVLETAPGVEEISGLPSGEVLET TAPGVDEISGLPSGEVLETTAPGVEEISGLPSGEVLETSTSAVGDLSGLPSGGEVLEISVSGVEDISGLPS GEVVETSASGIEDVSELPSGEGLETSASGVEDLSRLPSGEEVLEISASGFGDLSGVPSGGEGLETSASEVG TDLSGLPSGREGLETSASGAEDLSGLPSGKEDLVGSASGDLDLGKLPSGTLGSGQAPETSGLPSGFSGESS GVDLGSGPPSGLPDFSGLPSGFPTVSLVDSTLVEVVTASTASELEGRGTIGISGAGEISGLPSSELDISGR ASGLPSGTELSGQASGSPDVSGEIPGLFGVSGQPSGFPDTSGETSGVTELSGLSSGQPGVSGEASGVLYGT SQPFGITDLSGETSGVPDLSGQPSGLPGFSGATSGVPDLVSGTTSGSGESSGITFVDTSLVEVAPTTFKEE EGLGSVELSGLPSGEADLSGKSGMVDVSGQFSGTVDSSGFTSQTPEFSGLPSGLAEVSGESSRAEIGSSLP SGAYYGSGTPSSFPTVSLVDRTLVESVTQAPTAQEAGEGPSGILELSGAHSGAPDMSGEHSGFLDLSGLQS GLIEPS

GEPPGTPYFSGDFASTTNVSGESSVAMGTSGEASGLPEVTLITSEFVEGVTEPTISQELGQRPPVTHTPQL FESSGKVSTAGDISGATPVLPGSGVEVSSVPESSSETSAYPEAGFGASAAPEASREDSGSPDLSETTSAFH EANLERSSGLGVSGSTLTFQEGEASAAPEVSGESTTTSDVGTEAPGLPSATPTASGDRTEISGDLSGHTSQ LGVVISTSIPESEWTQQTQRPAETHLEIESSSLLYSGEETHTVETATSPTDASIPASPEWKRESESTAADQ EVCEEGWNKYQGHCYRHFPDRETWVDAERRCREQQSHLSSIVTPEEQEFVNNNAQDYQWIGLNDRTIEGDF RWSDGHPMQFENWRPNQPDNFFAAGEDCVVMIWHEKGEWNDVPCNYHLPFTCKKGTATTYKRRLQKRSSR HPRRSRPSTAH

K = lysine
H = histidine
R = arginine

Ala	a lanine
Cys	c ysteine
Asp	aspartic acid
Glu	glutamic acid
Phe	phenylalanine
Gly	glycine
His	histidine
Ile	<i>isoleucine</i>
Lys	lysine
Leu	leucine
Met	methionine
Asn	asparagi <mark>n</mark> e
Pro	p roline
Gln	glutamine
Arg	arginine
Ser	serine
Thr	threonine
Val	valine
Trp	tryptophan
Tyr	tyrosine
	Cys Asp Glu Phe Gly His Ile Lys Leu Met Asn Pro Gln Arg Ser Thr Val Trp