

3.052 Nanomechanics of Materials and Biomaterials: Spring 2007 Assignment #6

Due Date: Friday 05.11.07

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 any papers or podcast.

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

1. **Sacrificial Bonding in Biological Materials Podcast.** Fantner, et al. *Biophys. J.* **2006** 90, 1411.
 - a. Dr. Fantner comments that a modular structure with folded domains are not necessary for sacrificial bonding. Explain why. Where are the sacrificial bonds in Figure 3D?
 - b. In Figure 2, plots 2 and 3, Dr. Fantner explained that to create these simulated WLC curves, he used the same forces and same spacing between sacrificial bonds (i.e., A and B are always the same linear distance apart as you travel along the molecule). Why are the rupture distances for case 3 farther apart than those for molecule 2?
 - c. Is the increased energy dissipated in the systems described by Dr. Fantner with sacrificial bonding due to enthalpic contributions? Why or why not?
 - d. Consider a modular polymer with a fully unfolded contour length $L_{\text{contour}}(\text{unfolded})$ of 20 nm and a persistence length of 1 nm. Calculate and plot the normalized energy dissipated upon single chain stretching versus number of domains, N, from 0-20 where the contour length of each unfolded domain is $L_{\text{contour}}(\text{unfolded})/N$ and the rupture force = 200 pN. The energy normalization factor in the denominator should be for N=1. The most feasible way to complete this problem is by writing a code in Mathematica or Matlab.
 - e. Draw a schematic of an "ideal" force vs. distance curve for maximum energy dissipation involving sacrificial bonding, point out the different features of your schematic including where the sacrificial bonds rupture, and explain how they lead to increased energy dissipation.
 - f. Professor Zhibin Guan is a chemist at UC Irvine who has been designing synthetic polymers using the sacrificial bonding concept. Look up one of his papers on this topic and write a one paragraph summary (do not copy abstract).
 - g. Sacrificial bonding is thought to be particularly important to the fracture resistance of bone. Research the proposed molecular origin in the literature (i.e. which molecules and structures could be involved).
2. **Nanomechanics of DNA** (*data taken from Bustamante, et al., *Nature*, **2000**, 404,103).
 - a. Based on your knowledge of the structure of DNA, the electrostatic double layer, and of theoretical models for single molecule elasticity, how would you expect the global entropic chain stiffness (slope of force vs. distance curve) for stretching of a single DNA molecule to vary with salt concentration and why?
 - b. Below is a schematic and plot of optical tweezers data for stretching of double-stranded (ds) compared to single-stranded (ss)DNA. Explain all of the differences and similarities between the two curves.

Figure removed due to copyright restrictions.

See Figure 1 in Bustamante et al. *Nature* 404 (2000): 103.

c. The x-axis of the force vs. extension curve is given as “fractional extension” for dsDNA. How is it that “fractional extension” can be greater than one? Use this information to calculate the distance between adjacent base pairs in dsDNA in the two different structural forms depicted in the plot.

3. Nanoindentation of Seashell Nacre: Bruet, et al. *J. Mater. Res.* 20(9), **2005**. 2400-2419.

- a. Create two tables; one for fresh nacre and one for hydrated nacre. In each table, create columns with numerical values obtained from and calculated from data in the paper for P_{\max} , h_{\max} , and A_{\max} . P_{\max} is the maximum load upon indentation, h_{\max} is the maximum depth upon indentation, and A_{\max} is the projected contact area at P_{\max} and h_{\max} . You can assume that the Berkovich probe tip has an ideal shape.
 - b. Measure the RMS surface roughness of a real nacre sample using the AFM image which spans the full range of A_{\max} you obtained in 3a. Perform at least 50 measurements of different sizes. Plot RMS surface roughness (nm) vs. \sqrt{A} ($\sqrt{\text{nm}}$) and carry out a linear regression of this data.
 - c. Datasets of modulus values for each maximum load (calculated from the Oliver-Pharr method). Calculate and plot the coefficient of variation $\text{COV}(E) = \text{standard deviation}/\text{mean}$ for both fresh and hydrated nacre vs. the ratio $h_{\max}/\text{RMS roughness}$. Explain the resulting trends.
 - d. Describe the advantages and disadvantages of the finite element analysis (FEA) approach compared to Oliver-Pharr approach.
 - e. Explain the difference between Hardness values calculated from the Oliver-Pharr approach compared to AFM imaging measurements of residual indent area.
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