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3.22 Mechanical Properties of Materials  
Spring 2008

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## Problem Set #2

Due: Tuesday, March 4 by 5:00 PM

1. You did such an outstanding job in the engineering department at *Unique Unicycles* that they gave you a promotion to the R&D department. Your first assignment there is to study a new material developed by your competitors *Un-Unique Unicycles*. The material is a composite composed of unidirectional fibers in a polymer matrix (Fig. 1). While another research scientist determines what the fibers and matrix are made of, your boss Dr. Van Vliet asks you to determine the stiffness tensor components for such a structure in terms of Young's Modulus and Poisson's ratio.

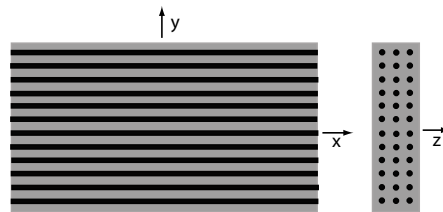


Figure 1: A composite material comprised of unidirectional fibers in a matrix.

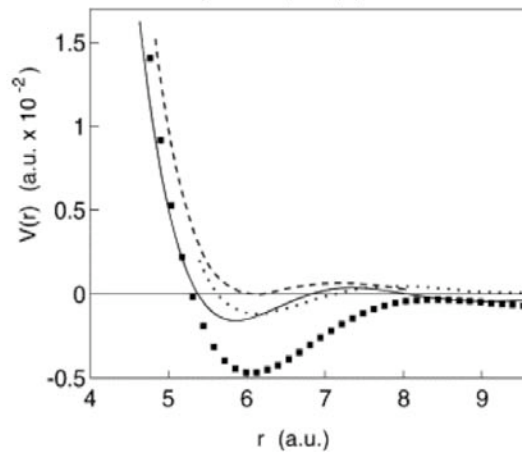
2. Two isotropic materials (A & B) are being considered for use in shoe insoles. When used as insoles the average strain with respect to time  $\epsilon(t)$  of the materials is that presented in the spreadsheet posted on the MIT Server (2-2.xls).
  - (a) Derive a model that accurately describes each material's response to the applied stress. Plot the result of your model and the given data.
  - (b) Characterize these materials, focusing on their elastic moduli and the relaxation time. Without having handled the materials, what class would each fall into?
  - (c) Which material is better suited for the job? Explain by showing the  $\sigma(t)$  (given that you take a step every second) and the resulting strain for each material. Define a quantity for judging the effectiveness of each material in this application. What would this quantity be for a material ideally suited for this application?
  - (d) A similar concept can be applied to measure the natural frequency of molecular chain rotation at the glass transition temperature of a polymer. Explain how you do this experimentally and the results you would expect.
3. You are responsible for performing uniaxial tensile tests on three very different materials: a 316 stainless steel alloy, alumina ( $\text{Al}_2\text{O}_3$ ), and high density polyethylene (HDPE). However, before performing the actual tests, you are asked to predict what the elastic stress vs. strain responses of each of the materials based on the mechanical properties of these materials documented in the literature (e.g., material property databases such as matweb.com, linked on the MIT Server.)
  - (a) Graph the engineering and true stress (MPa) versus engineering and true strain (%) response for all three materials on a single graph, up to an applied engineering strain value of .01 (or 1%) in strain increments of 0.0005.

- (b) Remark on the differences in behaviors seen for each of the three materials as related to their relevant mechanical properties. Also, looking at the magnitude of the stresses at the maximum applied strain, do you expect all of these materials to deform elastically up to these strains? If not, what was the fallacy in solely using Hooke's law to predict the stress-strain behaviors for each of the materials?
- (c) All three samples were given to you as cylinders with identical initial dimensions of 10 cm length and 2 cm diameter. Show whether a uniaxial load frame of maximum load capability = 100 kN (standard capabilities of load frames such as Instrons available at MIT) will be sufficient to deform all three materials to the requested engineering normal strain of 1%. Here, neglect the possibility that the materials might not remain intact (all in one piece) to that applied strain.
4. Atomic interactions can be modeled using a variety of potential energy approximations. One very common potential form is the Lennard-Jones 6:12 potential:

$$U(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$$

where  $\epsilon$  and  $\sigma$  are constants specific to a given material (note: these terms are NOT equivalent to stress and strain, but this is the standard notation for the L-J parameters). Here,  $r$  is the interatomic spacing given in units of Angstroms, and  $U(r)$  is given in units of eV atom<sup>-1</sup>. A molecular dynamics simulation was performed by Zhang and coworkers [1] to study the properties of Al thin films in which the authors proposed a Lennard-Jones potential of the form above to model Al-Al interactions. The values used for the material parameters were:  $\epsilon = 0.368$  and  $\sigma = 2.548$  (we've rounded off the values in the paper for your problem set).

- (a) What are the assumed units of  $\epsilon$  and  $\sigma$  in Zhang and coworkers' potential for aluminum?
- (b) Using the given material parameters and the form of the interatomic potential energy curve, plot  $U(r)$  for aluminum from  $r = 0$  to 3.5 Angstroms in increments of  $< 0.25$  Angstroms.
- (c) Determine the equation for and graph the interatomic forces  $F$  as a function of interatomic separation  $r$  for Al over the same range of  $r$  used in part (a), indicating units of  $F(r)$ . Also, analytically and graphically determine the equilibrium interatomic spacing,  $r_o$ . Mark this point on both the graphs produced in parts (a) and (b).
- (d) Compare this equilibrium interatomic spacing to the literature value of atomic radius for aluminum, and from that comparison explain what you think Zhang and coworkers assumed in choosing the constants  $\epsilon$  and  $\sigma$  that made  $r_o$  come out this way.
- (e) Figure 2 shows interatomic energy curves [ $V(r)$  is equivalent to our  $U(r)$ ] for Mg that were calculated by Chavarria [2] (squares) and McMahan and coworkers [3] (dotted and solid curve). These data are shown in arbitrary units (a.u.) which is typical of computational/experimental results that have funny units peculiar to the computational programming units, but  $r$  turns out to be expressed in  $\sim 2 \times$  Angstroms (i.e., 9 a.u. = 4.5 Angstroms). Comparing these curves with that calculated in part (a) for Al, explain whether you would expect magnesium to have a lower or higher elastic modulus than aluminum? Is this confirmed by the literature values of elastic properties and physical properties of Al and Mg?



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Figure 2: Interatomic potential for magnesium as calculated by Chavarria [2] (squares) and McMahan and coworkers [3] (dotted and solid curves).

- (f) Again, considering the relationship between the Young's modulus, the equilibrium interatomic spacing, and  $U(r)$  curvature, what effect do you think temperature has on the measured Young's modulus? Provide a conceptual explanation of your answer. (Hint: Think about what happens to atoms inside of a material as you heat it up.)

Refs:

1. H. Zhang and Z. N. Xia, Nuclear Instruments & Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 160 (2000) 372-376.
  2. G. R. Chavarria, Physics Letters A, 336 (2005) 210-215.
  3. A. K. McMahan and J. A. Moriarty, Physical Review B, 27 (1983) 3235-3251.
5. As discussed in lecture, the Worm Like Chain (WLC) model of rubber elasticity has been used to analyze the deformation of DNA under uniaxial loading. Bouchiat and coworkers used magnetic tweezers to extend lambda-DNA ( $\lambda$ -DNA) and applied the WLC model to infer its structure and resistance to bending. Table 1 is a subset of the experimental data Bouchiat and coworkers reported, with additional points (Bouchiat *et al.*, Biophys J. (1999) Fig. 2). Apply the WLC model to determine the following:
- (a) Graph these experimentally measured data as force on the chain vs. stretch of the chain,  $F_c$  vs.  $\lambda_c = r/r_o$  where  $r_o$  is the distance between chain ends before force is applied, and indicate the region over which the experimentally measured data is fit reasonably well by the WLC model.
  - (b) The number of nucleotides in this  $\lambda$ -DNA.
  - (c) The number of nucleotides that comprise a segment of the DNA that is significantly resistant to bending.
  - (d) The effective entropic spring constant of  $\lambda$ -DNA,  $k_s$ . Note that this is often defined as the resistance to extension at large forces – why is this? Compare your value to that

Table 1: A subset of the experimental data Bouchiat and coworkers reported, with additional points (Bouchiat *et al.*, Biophys J. (1999) Fig. 2)

Applied force $F$ (pN)	Extension $r$ ( $\mu\text{m}$ )
0.05	5.6
0.085	7.5
0.18	10.1
0.5	12.3
2.0	14.0
9.0	15.0

stated by the Bouchiat and coworkers, and explain why they expressed this stiffness in units of [N] instead of [ $\text{N m}^{-1}$ ].

- (e) The minimal force required to break the phosphate ester bonds that join nucleotides in DNA?
- (f) The stretch  $\lambda_c = r/r_o$  at which the WLC prediction diverges from that of the Freely Jointed Chain (FJC) model, by graphing the FJC prediction on the graph in (a), and the reasons for this divergence.