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ON THE USE OF CONTINUUM MECHANICS TO ESTIMATE THE PROPERTIES OF NANOTUBES

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On the use of continuum mechanics to estimate the properties of nanotubes

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§ **Abstract**

In the experimental and theoretical investigation of the properties of nanostructures, the equations of continuum beam theory are being used to interpret the mechanical response of nanotubes. In particular, Bernoulli-Euler beam bending theory is being utilized to infer the Young's Modulus. In this work, we examine the validity of such an approach using a simple elastic sheet model and show that at the nanotube scale the assumptions of continuum mechanics are no longer valid. Relations are derived for pure bending of nanotubes that show the explicit dependence of the "material properties" on system size.

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§1. Introduction

Recently, experimental methods have allowed for the measurement of the structural motion of nanometer scale objects [1-4]. In these works the notions of continuum mechanics have been used to infer that carbon nanotubes possess super-high Young's moduli. Other theoretical work using direct atomic simulation [5] has also reached similar conclusions. In [5], for instance, a comparison of bending stiffnesses was made between a C_{200} single-wall nanotube and an Iridium beam of "similar dimensions". The bending stiffness of the carbon nanotubes was determined from a simulation of the atomic structure using the Keating potential; the bending stiffness of the Iridium beam was deduced using the continuum Bernoulli-Euler theory of beam bending. This type of comparison or data interpretation, however, must be done carefully since the continuum hypothesis is being pushed to its limits – as has been previously acknowledged [4,5]. In this paper, we show by using a highly idealized elastic sheet model for a nanotube that the observed super-high Young's moduli are direct consequences of the breakdown of the continuum hypothesis. Further it is shown that the scale at which the continuum hypothesis breaks down is a function of the mode of deformation utilized to determine the mechanical properties.

§2. Young's Modulus

The Young's Modulus, E, of a material is defined as the ratio of the normal stress, $\sigma = F/A$, to the normal strain, $\varepsilon = \Delta/L$, in a 1-dimensional tension test; see Fig 2.1(a), where F is the applied force, A is the cross-sectional area of the specimen, Δ is the specimen elongation, and L is the specimen length. Thus,

$$E = \frac{\sigma}{\varepsilon} = \frac{FL}{A\Delta}. \tag{2.1}$$

The definition relies on the continuum hypothesis and is designed such that E is truly a material property. In other words, the definition of E is designed so that regardless of specimen geometry, A or L, the value of the Young's Modulus is invariant for a given material. Note that other modes of deformation can be used to define the Young's Modulus. However, independent of deformation mode, E is the same constant for a given material. For example, in a beam bent by a pure moment, with a large aspect ratio (greater than approximately 10), the Young's modulus can be defined by

$$E = \frac{ML}{I\theta}, \tag{2.2}$$

where M is the moment applied to the beam, I is the area moment of inertia of the beam cross-section, θ is the rotation of the end section of the beam, and L is the length of the beam; see Fig. 2.1(b).

In both definitions, one assumes that all the displacements (relative to the beam length) and displacement gradients are small. Further the cross-sectional properties are the properties of the cross-section when it is treated as a continuum; ie. one counts the

space between atoms. The assumptions behind these definitions of Young's modulus are valid at the macroscopic scale where they are typically utilized in engineering applications. The definitions, however, break down as definitions of a *material property* (something intrinsic to the material) as the specimen sizes decrease to the atomic scale. The rate of breakdown is dependent on the mode of deformation used to define E.

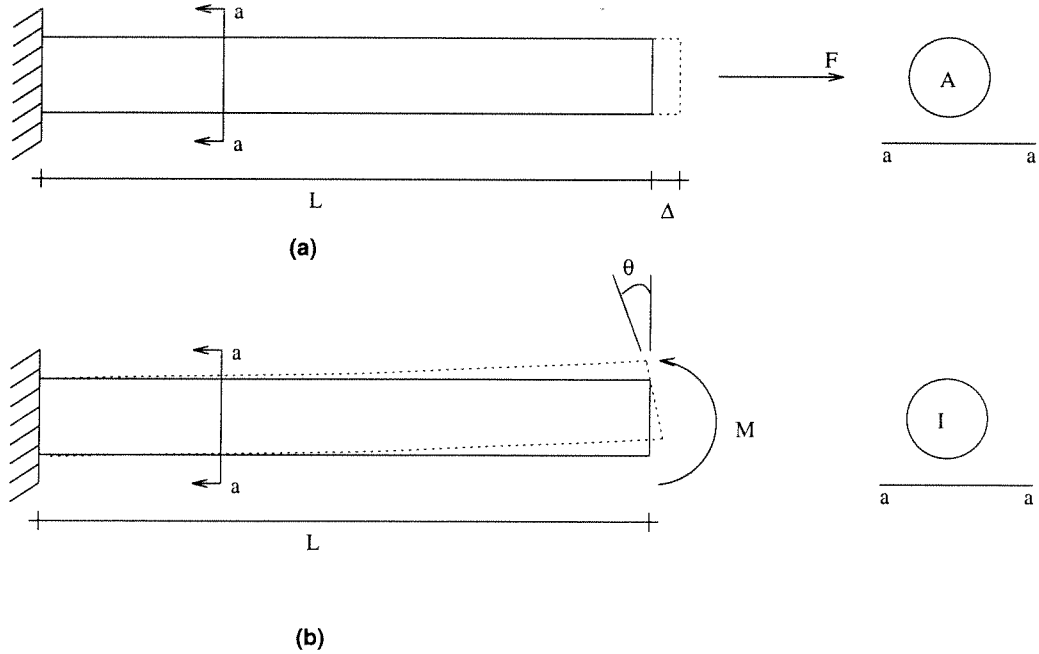

FIGURE 2.1. Geometry, motion, and load used to define Young's Modulus. (a) axial extension; (b) pure bending.

§3. Pure Bending

Consider a beam of length L under pure bending (no transverse shear). The beam is made up of n tubular sheets of atoms that are spaced a distance s apart. The thickness of each sheet is t and the distance to the center of sheet j is denoted R_j. Thus the inner radius of the beam is $R_1 - t/2$ and the outer radius is $R_n + t/2$. The mean radius of any sheet can be expressed as $R_j = R_1 + (j-1)(s+t)$; see Fig 3.1. Assume further that $L > 10R_n$ so that the Bernoulli-Euler kinematic assumption is valid; ie. the motion of the material is dominated by the rotation of the beam cross-sections which remain planar and orthogonal to the central axis of the beam. It is also assumed that all sheets have the same end rotation. For the imposed loading, this gives a deflected beam whose central (neutral) axis has constant curvature equal to θ/L where θ is the rotation of the cross-section at the tip of the beam. Each individual sheet has a mono-layer of atoms which we assume does not interact with neighboring sheets. For this problem, elongation dominates the behavior; thus, the important material property of each sheet will be the axial stiffness per unit angular distance. For simplicity we assume this property to be the same constant E^* for each sheet. Note that E^* essentially depends on nature of the atomic bonding

in an individual sheet which we assume to be the same over a reasonable range of sheet curvatures.

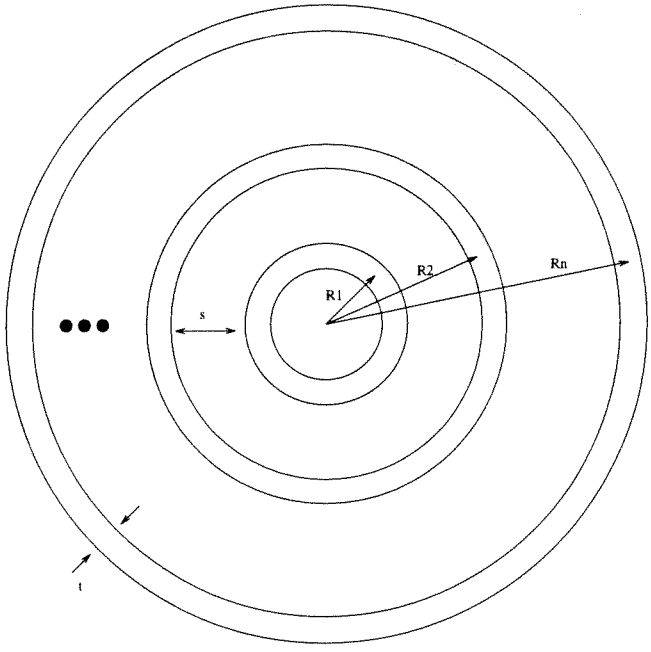

FIGURE 3.1. Cross-sectional parameters for a multi-walled nanotube.

Let us first examine a single sheet j. Under the action of bending, the end cross-section of the sheet will rotate an amount θ. Thus we find from elementary strength of materials that the moment M_j in sheet j is given as

$$M_j = E^* \pi R_j^3 t \frac{\theta}{L}\,, \tag{3.1}$$

where for simplicity we have assumed that $t << R_j$ and ignored terms $O(R_j^{4-l}(t/2)^l) \quad l \in \{2,3,4\}$.

Thus, for a total applied moment M, sheet j will carry a moment of

$$M_j = \frac{R_j^3}{\sum_{i=1}^n R_i^3} M\,. \tag{3.2}$$

Substituting Eq. (3.2) into Eq. (3.1) gives the "moment-curvature" relation

$$M = E^* \pi t \left(\sum_{j=1}^n R_j^3 \right) \frac{\theta}{L}\,, \tag{3.3}$$

where θ/L is the curvature of the bent beam for our special load case. If we now apply definition (2.2) with (3.3), we get an apparent Young's modulus of

$$\widehat{E}(n) = E^* t \frac{\pi \sum_{j=1}^n R_j^3}{I}\,, \tag{3.4}$$

where I is the area moment of inertia of the gross section; ie. $I = \frac{\pi}{4}[(R_n + t/2)^4 - (R_1 - t/2)^4]$.

The true Young's modulus, denoted E, of the material is given from Eq. (3.4) in the limit $n \to \infty$. As one could have initially guessed, this gives $E = E^* t/(s+t)$; ie. the sheet stiffness averaged over the space allotted to an individual sheet in a continuum body. We can define a non-dimensional measure of the departure from the continuum hypothesis as

$$\bar{E} = \frac{\widehat{E}}{E} = \frac{4(1 + t/s)\sum_{j=1}^{n}(R_j/s)^3}{(R_n/s + \frac{1}{2}t/s)^4 - (R_1/s - \frac{1}{2}t/s)^4}\,. \tag{3.5}$$

If we consider the special case of $t << s$ then we have that

$$\bar{E} \approx \frac{4\sum_{j=1}^{n}(R_1/s + (j-1))^3}{(R_1/s + (n-1))^4 - (R_1/s)^4}\,. \tag{3.6}$$

Remark 3.1.

It can easily be seen for this mode of deformation that an experiment on a nanotube of only a few sheets of atoms will yield a much higher apparent value of the Young's modulus than the continuum value. Using Eq. (3.6) for example, we have with $n = 2$ and $R_1/s = 2$ that $\bar{E} \approx 2.15$. The issue of importance, however, is that the continuum hypothesis is no longer valid, not that the modulus of the material doubles at small scales. □

Remark 3.2.

The approach to the continuum limit in Eq. (3.5) is governed by the ratio of two 4th order polynomials. In the special case where $t << s$ and $R_1 = 0$ (a solid beam), Eq. (3.6) gives $(n/(n-1))^2$; in particular we need $n > 201$ for the validity of the continuum hypothesis, which we define here as the condition $0.99 < \bar{E} < 1.01$. □

Remark 3.3.

Cantilevered nanobeams acting under an end shear force will have a slightly different expression for the apparent Young's modulus. However, for structures with a large aspect ratio (length to diameter greater than 10) one will again recover Eq. (3.5). □

Remark 3.4.

The limits of integration that one chooses when defining I play a crucial role in the break down of the continuum limit. From Eq. (3.4), we see that the controlling factor on the validity of the continuum hypothesis rests on the convergence of the Riemann sum in the numerator to the integral in the denominator. This is more easily seen by rewriting this expression as

$$\widehat{E}(n) = E\frac{(s+t)\sum_{j=1}^{n} R_j^3}{\int_{\alpha}^{\beta} r^3\, dr}\,, \tag{3.7}$$

where α and β are the inner and outer radii of the nanobeam. The Riemann panel area is thus seen to be $s+t$ and the sum involves n Riemann panels. The precise definition of α and β clearly has a large influence on the computed value of $\widehat{E}(n)$. To be more faithful to the Riemann sum, one should define the gross section properties using $\alpha = R_1 - t/2 - s/2$ and $\beta = R_n + t/2 + s/2$. The modification leads to a faster convergence to the continuum limit. Thus in the processing of experimental data for $\widehat{E}(n)$, it is imperative to use a definition of I that leads to the fastest approach to the limit in order to more accurately determine E, the true Young's modulus of the material. For example if $R_1/s = 2$, $n = 2$, and $t << s$, then with the modified definition of the area moment of inertia we have $\bar{E} \approx 0.97$; (compare to $\bar{E} \approx 2.15$ from above). □

Remark 3.5.

In axial extension, if the cross-sectional area is defined to include a half inter-sheet spacing added to the outer and inner radii, then $\bar{E} = 1$ independent of n. This occurs because the important measure of the cross-section in extension is the cross-sectional area and the Riemann sum of a constant (unity) is exact. □

§4. Conclusions

1. In this report, we have derived approximate formulas for the determination of the break down of the continuum hypothesis. In particular we have shown that for nanobeams in bending, one needs more than 201 atomic layers for the validity of continuum notions such as Young's Modulus. Thus the interpretation of experimental data on nanostructures through the reporting of apparent continuum properties can be somewhat misleading.

2. More accurate processing of experimental data can be effected by modifying the definitions of the cross-sectional properties. Thus by increasing the outer boundaries of a specimen by half of the inter-atomic sheet spacing the true Young's modulus of the material can be more closely determined.

3. Through a system identification process one could also take the collected data for the product $I\widehat{E}$ and determine the parameters E^* and t.

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