Deformations of adhering elastic tubes

K. Tamura*, S. Komura* and T. Kato*

*Department of Chemistry, Tokyo Metropolitan University, Tokyo 192-0397, Japan

Abstract. Deformation of an elastic tube adhering onto a substrate due to van der Waals attractive interaction is investigated by means of computer simulation and scaling theory. The sum of the stretching, bending, and van der Waals energies of the tube is numerically minimized using the conjugate gradient method. The onset of the deformation and the total energy can be scaled with a variable C_b/N^2, where C_b is the bending constant and N the size of the tube. For a significantly deformed tube, the scaling relation between the bending energy and the bending constant is explained within the shell theory.

INTRODUCTION

Carbon nanotubes have attracted great interests due not only to their peculiar structure, but also to the electrical, chemical, and mechanical properties associated with these structures. Examples of the possible applications are such as nanowires or electronic devices. The electric transport through nanotubes is studied after their deposition on a substrate with which they interact. It is known, however, that the resistivity of the nanotube is affected by their elastic deformations. Since there is little control over the alignment and the shape of adsorbed nanotubes, it is crucial to know how they deform on the substrate. There are several works which report on the deformations of nanotubes due to the van der Waals (vdW) interaction. Multiwalled nanotubes can even fully collapse along their length [1, 2].

In this paper, we theoretically investigate the deformation of an elastic nanotube adhering onto a rigid substrate due to the vdW attractive interaction.

MODEL AND RESULTS

Consider a cross section of an elastic tube interacting with a rigid substrate. We assume that the axial deformation is uniform along the tube. The elastic tube is modeled by a circular network of N beads connected by harmonic springs. The adhesion energy is taken into account through the vdW interaction between each of the bead and the substrate.

The discretized stretching energy is given by the sum over Hooke's law of each spring:

$$E_s = \sum_i \frac{1}{2} C_s \left(\frac{L_i - L_0}{L_0} \right)^2 . \quad (1)$$

FIGURE 1. Equilibrium configurations of the deformed tubes for various values of the scaled bending constant $c_b = C_b/\varepsilon$. The tube globally flattens for $c_b = 0.1$, but hardly deforms for $c_b = 1000$.

Here, C_s is the spring constant, L_i is the length of the i-th spring, and L_0 is the natural length of the spring taken here as a constant. The discretized bending energy, on the other hand, is calculated by

$$E_b = \sum_{\langle ij \rangle} \frac{1}{2} C_b |\hat{n}_i - \hat{n}_j|^2 , \quad (2)$$

where C_b is the bending constant, $\hat{n}_i$ is the unit normal vector of the i-th spring, and the sum is taken over each pair of springs which share a common bead. The adhesion energy of the tube is taken into account through the vdW interaction between each of the bead and the substrate:

$$W = \sum_i \frac{2^{8/3}}{3} \varepsilon \left[\left(\frac{\sigma}{z_i} \right)^{12} - \left(\frac{\sigma}{z_i} \right)^{3} \right] , \quad (3)$$

where z_i is the height of the i-th bead from the substrate. When the adhesion energy per bead is plotted against z_i, ε corresponds to the depth of the energy minimum.

The total energy $E_{tot} = E_s + E_b + W$ is numerically minimized in the computer using the conjugate gradient method. As for the initial condition of the simulation,

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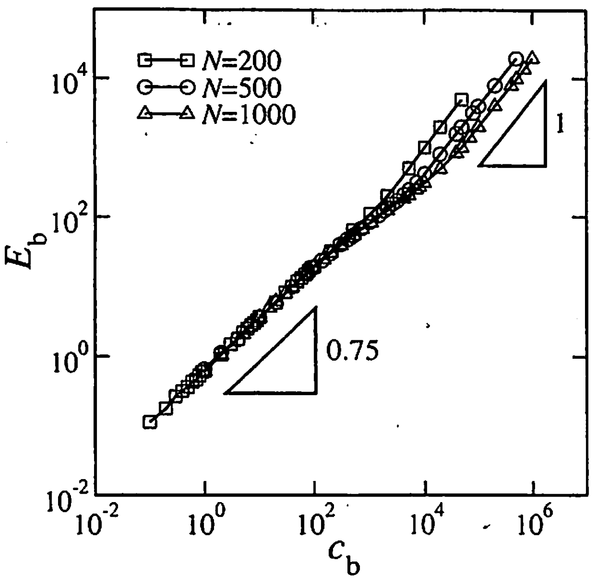

FIGURE 2. The bending energy E_b as a function of c_b for size $N = 200, 500, 1000$. We see two scaling behaviors: $E_b \sim c_b/N$ and $E_b \sim c_b^{0.75}$ for large and small c_b, respectively.

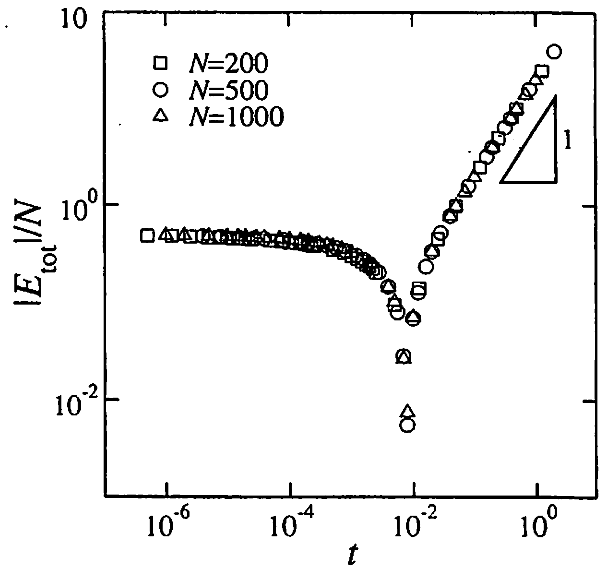

FIGURE 3. The absolute value of the total energy per bead $|E_{tot}|/N$ as a function of the scaling variable $t = c_b/N^2$. The scaling $E_{tot}/N \sim t$ holds in the "bending regime", whereas E_{tot}/N asymptotically approaches to -1 in the "adhesion regime".

each bead is located on a circle with a distance being equal to the natural length of the spring L_0. Since there is no spontaneous curvature in our model, even the undeformed tubes cost certain curvature energy.

In equilibrium, each spring relaxes almost at its natural length. For a large bending constant such as $c_b = 1000$, the tube hardly deforms and keeps its circular shape in spite of the adhesion. As c_b is reduced to $c_b = 10$, a considerable deformation occurs and the contact area (line) increases significantly. Further decrease of c_b results in a configuration such as $c_b = 0.1$ in Fig. 1. Here a flattening of the tube is observed, and the curvature is localized at the regions close to the contact line.

For almost undeformed tubes on which the curvature is uniformly distributed, the bending energy can be readily estimated. Since the radius of curvature is proportional to the number of beads N in such a case, the bending energy becomes $E_b \sim N(C_b/N^2) \sim C_b/N$. This linear dependence of E_b on C_b in the undeformed region can be checked in Fig. 2 where we have plotted E_b against C_b. For smaller c_b, on the other hand, all the data collapses on a single straight line regardless of the tube size N. In this strongly deformed region, we observe a nontrivial scaling behavior, i.e., $E_b \sim c_b^{0.75}$. This nontrivial scaling can be understood within the shell theory.

When a tube of radius R is largely deformed on a substrate, a contact area develops. For such a deformation, the elastic energy is localized in the two parallel straight strips near the edge of the bulge. We apply the argument of Ref. [3] for a tube, and the total elastic energy becomes

$$E_b \sim \left(\frac{C_s}{L_0^2}\right)^{1/4} C_b^{3/4} \frac{H}{R^{3/2}}, \qquad (4)$$

where H is the depth of the bulge being fixed and given. The scaling relation Eq. (4) accounts for the dependence of E_b on C_b as seen in Fig. 2. Notice that, in our simulation results, the contribution of the equilibrated stretching energy E_s is negligibly small compared to that of other energies, i.e., $E_s + E_b \approx E_b$.

In Fig. 3, we have plotted the absolute value of the total energy per bead $|E_{tot}|/N$ as a function of $t = c_b/N^2$ for three different tube sizes. Notice that E_{tot} can take negative value due to the vdW interaction when the tube is strongly adsorbed. It is remarkable that all the data collapse onto a single curve irrespective of the tube size N. Hence the total energy can be scaled with c_b/N^2.

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