A MODEL OF NANOSCALE FRICTION BETWEEN A CARBON NANOTUBE AND A SUBSTRATE

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Summary It is well-known that nanoscale friction between, for example, a carbon nanotube and a substrate, differs significantly from its macroscale counterpart. In this paper a structural mechanics model, which includes the effects of extensibility and shear deformation in the slip and stick regions, is shown to predict a maximum friction force which does not vary for substrate widths less than a critical value. The results from this model provide a quantitative explanation of previous experiment work in the literature.

INTRODUCTION

It is known that friction at the nanoscale differs significantly from its macroscale counterpart. In particular Whittaker *et al.* [1] conducted an experimental investigation of friction between a single-walled carbon nanotube and a silicon dioxide substrate. The nanotube was suspended over a trench and an AFM was used to push the nanotube toward the bottom of the trench (Fig. 1). The force required to induce sliding over the substrate was determined and related to the tensile force in the nanotube. It was found that the critical force in the CNT required to induce sliding was about 8 nN. Surprisingly this value was independent of the width of the substrate for widths up to approximately 230 nm. In a subsequent study, McElroy *et al.* [2] investigated the effects of wider substrates (230 to 850 nm) and found a nearly linear increase in friction force with width in that regime. However no casual explanation of this unexpected behaviour was presented in either study.

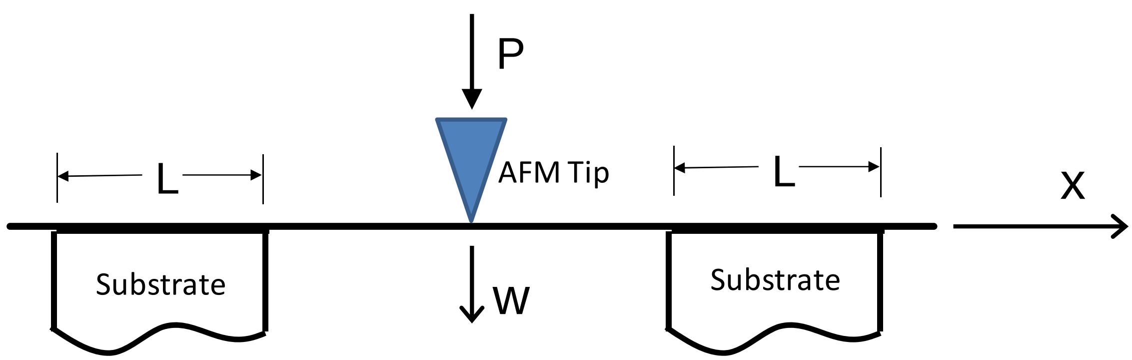

Figure 1. AFM tip pushing down on a suspended CNT so as to induce sliding as in [1] and [2].

Recently Ryan *et al.* [3] showed that the one-sided nature of a bonded constraint can lead to significantly different behaviour than that for a double-sided bond (Fig. 2). This behaviour is due to a combination of extensional and shear deformation in the bonded region. In the case studied the inclusion of these effects leads to a finite stiffness at what would otherwise be considered a “fixed” support. In another recent work Majidi and Adams [4] developed a simple method for modeling the effect of adhesion. Essentially the unknown contact dimension can be found using a boundary condition which specifies the discontinuity in bending moment, shear, and axial force. This boundary condition automatically satisfies energy minimization and thus significantly reduces the algebraic complexity involved in solving such problems.

In this paper we present a structural mechanics model, which includes the effects of extensibility and shear deformation in the slip and stick regions. The initially unknown location of the stick-to-slip boundary is determined using the method of [4]. It is shown that this model predicts a constant maximum friction force for substrate widths less than a critical value. This critical value depends on the work of adhesion between the nanotube and substrate as well as on the nanotube modulus and cross-section dimensions. The results from this model provide a quantitative explanation of previous experiment work in the literature [1]-[2].

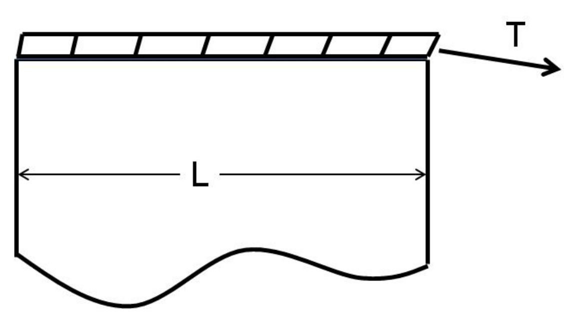

Figure 2. Expanded view of CNT lying on the substrate with the rotations of cross-sections shown.

MODEL

Consider the equations for cross-section rotation (ψ), transverse and axial displacements (w,u) in beam theory

$$\frac{d}{dx}\left[\kappa^2 GA\left(\frac{dw}{dx}+\psi\right)\right]+p=0, \qquad \frac{d}{dx}\left(EI\frac{d\psi}{dx}\right)-\kappa^2 GA\left(\frac{dw}{dx}+\psi\right)+T\frac{dw}{dx}=\frac{qh}{2}, \qquad \frac{d}{dx}\left(EA\frac{du}{dx}\right)=-q \tag{1}$$

where κ^2 is the shear correction factor, E and G are the elastic and shear moduli respectively, p and q are the distributed loads per unit length acting on the lower surface in the transverse and axial directions respectively, and I is the second moment of the cross-section of area A and height h.

In a stick region $w = 0$ and $u = (h/2)\psi$, whereas in a slip region $w = 0$ and $q = -\tau b$, where τ is the shear stress and b is the cross-section contact width which varies from about 5% (multi-walled CNT) to 50% (single-walled CNT) of the diameter [5]. These conditions can be used to simplify Eq. (1) leading to

$$\text{Stick Region}: \; E(I+Ah^2/4)\frac{d^2\psi}{dx^2}-\kappa^2 GA\psi=0, \; -L<x<-a, \quad \text{Slip Region}: \; EI\frac{d^2\psi}{dx^2}-\kappa^2 GA\psi=-\tau bh/2, \; -a<x<0 \tag{2}$$

The solution of these ordinary differential equations in the stick and slip regions is straightforward. However special care needs to be taken when using boundary and continuity conditions. The result is one nonlinear algebraic equation which relates the maximum friction force to the length of the substrate for different values of the work of adhesion and shear stress.

RESULTS

Although the results can be presented in nondimensional form, in order to facilitate comparison with [1] and [2] the results are given in dimensioned form in Fig. 3 for axial force required for complete slip vs. contact length. These results give a sliding force of about 8 nN (narrow substrates) with a linear increase (wider substrates) which, for a work of adhesion of 7 mJ/m^2 and a shear stress of 30 MPa, agrees well with the experimental work in [1] and [2].

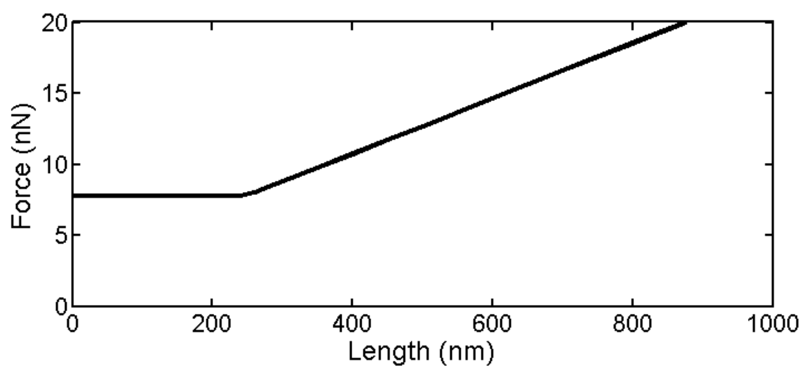

Figure 3. Axial force applied to nanotube required to produce sliding vs. contact length.

CONCLUSIONS

Nanoscale friction between a carbon nanotube and a substrate differs significantly from its macroscale counterpart. In particular below a critical substrate width the maximum friction force is independent of the width; for wider substrates the friction force increases almost linearly. A structural mechanics model, which includes the effects of extensibility and shear deformation in the slip and stick regions, is shown to correctly predict this unexpected behaviour of the maximum friction force. The critical value of the width depends on the work of adhesion between the nanotube and substrate as well as on the nanotube moduli and cross-section dimensions.

References

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