EFFECTIVE SIMULATION APPROACH FOR STUDY OF CARBON NANOTUBE MECHANICAL PROPERTIES

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Abstract

We present the novel, effective, and simplified methodology to simulate and investigate physical properties of vertically aligned multiwall carbon nanotubes (MWCNTs), the mechanical properties in particular. Unlike conventional solutions, we consider nanotube as a beam with a fixed end and a free end, allowing us to employ the mechanics of beam used as cantilever. Considering the atomic force microscopy (AFM) force-distance measurement as possibility to experimental determination of CNTs mechanical properties, we simulated the interaction of carbon nanotube structure with AFM cantilever at the applied force. We investigate the effect of inner and outer radius, different values of Young's modulus, and various lengths of MWCNTs. The methodology, we present, is a significantly quick simulation approach providing validate information about MWCNTs mechanical behavior.

Keywords: Multiwall carbon nanotubes, mechanical properties, Young's modulus, beam, AFM,

1. INTRODUCTION

The physical properties of carbon nanotubes (CNTs) have been predicted to be outstanding and to have high potential for wide spread application since their discovery [1]. Mechanical properties of CNTs are exceptional and crucial, for instance, in the field of flexible electronics (electronic paper, wearable displays, smart gloves and so on) [2-5]. It was estimated earlier by Yu et al. that CNTs have extremely high Young's modulus in the range of hundreds of GPa or even higher [6,7]. However, experimental verification of predicted value still remains unsolved. The experimental evaluation of these properties has become to be a challenging task due to circumstances such as small CNTs diameter, and difficulties with CNTs manipulation. Nevertheless numerous different methods (especially using atomic force microscopy (AFM) often combined with nanoindentation) have been reported [2-7]. The atomic force microscope (AFM) has been used later on and the stiffness was derived from tip-tube interaction force curve [8]. Furthermore, the scientists have combined AFM technique with an independent determination of CNT structure obtained by using thin carbon grid membranes. In the development of these measurement methodologies the simulation is necessary tool. There has been published many approaches to do so, often considering the different point of views.

The approach we present, is significantly quick, simply, simulation providing validate information about CNTs mechanical behavior. The study of CNTs behavior is done for different CNTs geometries and different CNTs tensile modulus (Young's modulus). This solution could help in development of more effective experimental measurement of CNTs mechanical properties.

2. SIMULATION METHODOLOGY

The mechanical properties simulation is based on the fact that the CNT structure is considered as beam with one fixed end and one end free. The methodology of the simulation is described below. The bending can be simulated using the following differential equations (1,2):

$$EI\frac{d^2y}{dx^2} = M\ , \tag{1}$$

$$\frac{d^2M}{dx^2} = F_x\delta(y - Y_{end}) + F_y\delta(x - X_{end}), \tag{2}$$

with boundary conditions (3) of:

$$y\big|_{x=0} = 0 \qquad \left.\frac{dy}{dx}\right|_{x=0} = 0 \qquad M\big|_{x=X_{end}} = 0\ , \tag{3}$$

where *E*, *I* and *M* are Young's modulus, moment of inertia of the nanotube under scrutiny and moment of bending. For a hollow cylindrical beam with outer and inner radius R_1 and R_2, respectively, the moment of inertia *I* can be calculated by the following equation (4):

$$I = \iint_S y^2 dxdy = \frac{1}{4}\pi\left(R_1^4 - R_2^4\right), \tag{4}$$

In order to solve the differential equations (1,2), the coordinates (X_{end}, Y_{end}) of the free end have to be known first. Since this condition is not fulfilled, another constraint that the length of the nanotube keeps unchanged is applied this question (5) where *L* is length of CNT structure.

$$\int_0^{X_{end}} \sqrt{1 + \left(\frac{dx}{dy}\right)^2}\, dx = L \tag{5}$$

The differential equations are then solved by the iteration method. Following the roadmap given below, the coordinates of the free end are obtained at an applied force *F*.

1. For a given *Xend*, the *Yend* value is estimated and the differential equation is then solved using Adams-Moulton's method.
2. Output *Yend* and input *Yend* are compared. If the relative error is greater than predefined value, new *Yend* through bisection method is estimated and step 1 is repeated. Once the relative error is within the predefined range, step 3 is applied.
3. Based on the *Xend* and *Yend*, the length of the bent CNT by Gauss quadrature rule is calculated. If the relative error is greater than a predefined value, another *Xend* is estimated and step 1 is repeated. Otherwise, *Xend* and *Yend* are recorded.

After obtaining (X_{end}, Y_{end}) at the given force, the applied force is increased by a predefined step-value; a pair of new free coordinates is calculated using the same method.

In AFM, the curve obtained is force against sample displacement, which is equal to (6)

$$Z = (L - X_{end}) + Y_{end} \sin\theta + kF \,, \tag{6}$$

where *k* is the spring constant of the cantilever. Analytically, the hollow tube deflection *D* can be described by the mathematical formula:

$$D = \frac{FL^3}{3EI} \,. \tag{7}$$

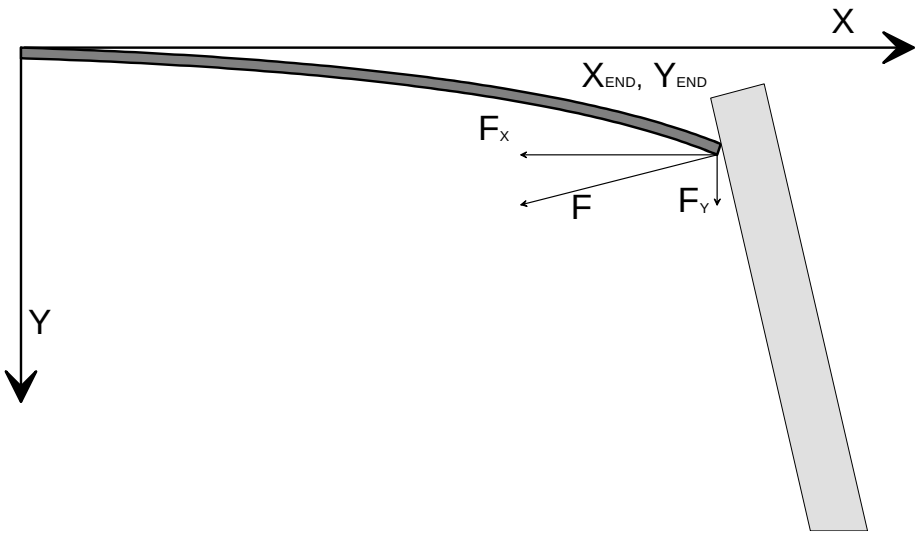

Fig. 1 Schematic representation of interaction of AFM cantilever and CNT structure. Horizontal bent structure represents the CNT while the bar represents the cantilever.

3. RESULTS AND DISCUSSION

The method was verified by running a number of simulations with one quantity as parameter. We have also used this method to empirically created relationship between the CNT cantilever interaction and CNT mechanical parameters to help us later on with derive those parameters.

3.1. The interaction between cantilever and CNTs

As we explained above, the simulation is done to be used in future to help the actual measurement and determination of CNTs mechanical properties. The Figure 2 shows the interaction between cantilever and CNTs as it would be result shown performing the force spectrum measurement. The parameter of CNTs is length of 30 μm length and diameter of 30 μm and 300 nm, respectively. The Young's modulus of CNT was assumed to be 500 GPa.

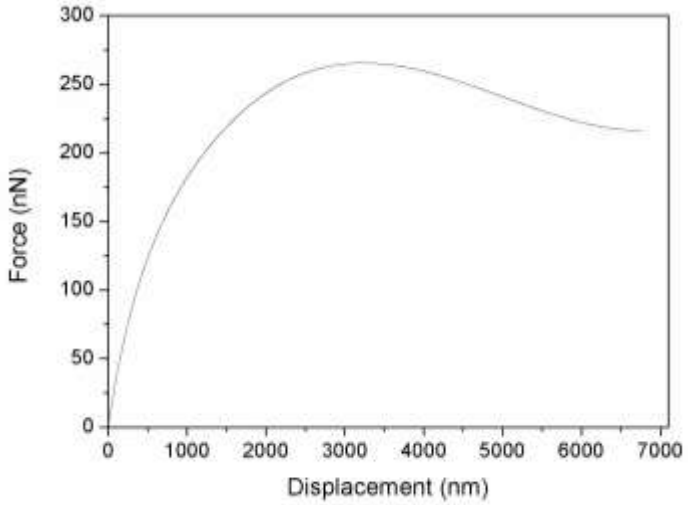

Fig. 2 The simulation of force distance curve formed by interaction between CNT and AFM cantilever. The CNT structure with parameters: length and diameter of 30 μm and 300 nm, respectively. The Young's modulus of CNT was assumed to be 500 GPa.

3.2. Various CNTs parameters

First we simulated cases with constant CNT length of 30 μm, inner (100 nm) and outer (200 nm) diameter and E as parameter (see Figure 3). Important result from this simulation was finding that the first derivative of the bending in origin (first contact with the cantilever) is linearly proportional to the amplitude of Young's modulus. Constant CNT inner and outer diameters, Young's modulus and variable length *L* (see Figure 4). Here we observed that the slope during first contact (initial force) is linearly proportional to $1/L^3$. Finally we have simulated constant CNT length and its Young's modulus with variable outer and inner diameter keeping the wall thickness constant (see Figure 5). Here we observed that the force is linearly proportional to the cube of CNT outer radius. All results are corresponding to the Eq. (6) thus verifying the simulation model was created correctly.

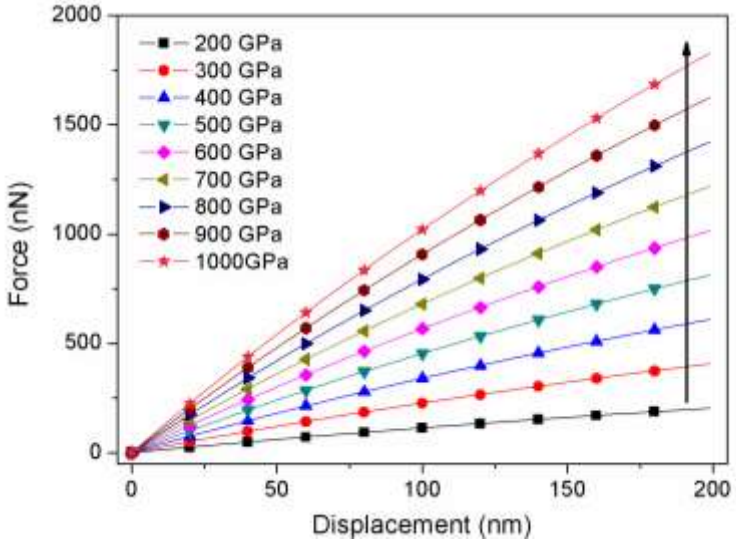

Fig. 3 The force-distance simulation where the Young's modulus of CNT is a parameter. The length of CNT is 30 μm, inner and outer radius is 100 nm and 300 nm respectively. The interaction is assumed to be with one CNT in contact at once.

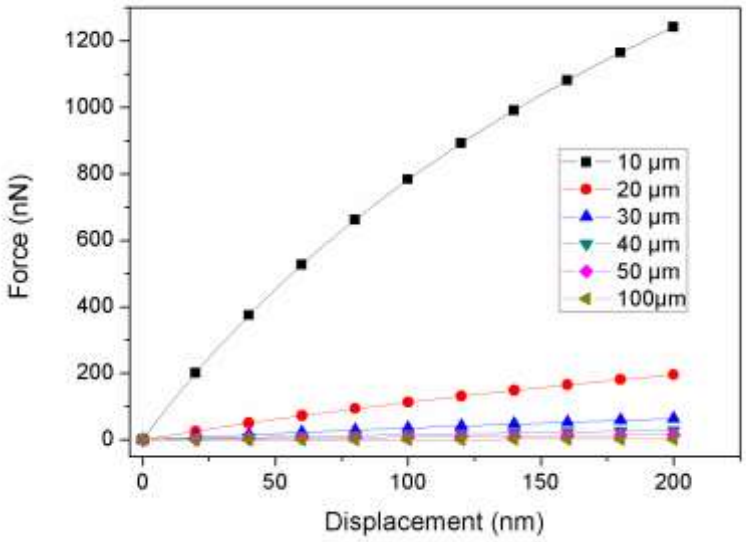

Fig. 4 The force-distance simulation where the length of CNT is a parameter. The Young's modulus of CNT is set to be of 500 GPa. The interaction is assumed to be with one CNT in contact at once.

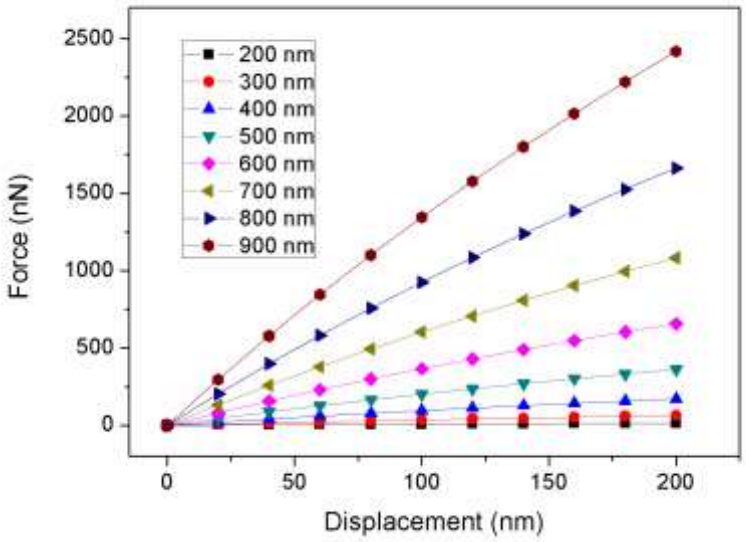

Fig. 5 The force-distance simulation where the outer diameter of CNT is a parameter. The length of CNTs is 50 μm. The Young's modulus of CNT is set to be of 500 GPa. The interaction is assumed to be with one CNT in contact at once as it was in all previous cases.

CONCLUSION

In this paper we proposed the effective simply way to simulate the mechanical properties of vertically aligned multiwall carbon nanotube. The method is based on consideration of nanotube structure as cylinder beam with one end fixed. We simulated the CNTs with different inner and outer radiuses, respectively, different lengths, and different values of Young's Modules. The method we proposed could be seriously employed for experimental determination of the mechanical properties. In case of using this simulation methodology the measurement is to probably be simply effective with significant results as well.

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