

3-D Modeling of a Carbon Nanotube Cantilever Biosensor

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Abstract—In this paper, 3-D finite element modeling and simulations are carried out to investigate the bending deformation of a single-walled carbon nanotube cantilever biosensor due to mass attached, and addition of a nano-scale particles to the beam tip resulting from the bioparticle detection. In addition, an algorithm for an electrostatic-mechanical coupled system is developed. The computed results are in excellent agreement with the well known electrostatic equations that govern the deformation.

I. INTRODUCTION

The development of nanoscale technologies in recent years has enabled exciting possibilities for biological sensing. The devices that can be developed with nanoscale materials allow biological sensing of very small concentrations of target molecules offering better sensitivities than conventional biosensing devices. Among the enabling nanostructures, carbon nanotubes (CNTs) are unique and have emerged as a new platform due to their interesting electrochemical and electrical properties including varying electrical property (from metallic to semiconductor), small diameters, high mechanical strength, good conductivity and ease of fabrication and integration.

Among several developed CNT biosensing approaches including CNT-FET [1], liquid suspension system [2], and CNT forest, CNT cantilever [3] has produced a great deal of interest because of its low cost, high sensitivity, ease of fabrication, and label free detection. The CNT cantilever undergoes a change in its mechanical properties upon the binding of target biomolecules due to a differential surface stress caused by the explicit adsorption on its surface. In fact, in response to any chemical, physical or environmental factors, it produces an equivalent mechanical motion in the nanometer scale. However, depending on the mechanical property of the device, the sensing method of the motion, e.g. capacitance, piezoresistance or resonance frequency, can vary. Also, the parameters used for measuring the motion can be either cantilever bending (deflection mode) or shifts in resonant frequency (resonance mode). A cantilever can be used in several other sensing applications including gas sensing, pH sensing, DNA hybridization, liquid sensing, and

protein detection. Knowles et al. [4] developed a microcantilever system for protein accumulation where the surface stress generated by the interaction between the protein and the beam was used to detect the protein. Li et al. [5] designed a cantilever array with receptor molecules to simultaneously detect cancer and cardiac markers.

The sensitivity of the cantilever biosensor is greatly influenced by its surface functionalization, and its selectivity is accomplished by immobilizing specific receptors on the top surface of the cantilever. Unlike other cantilever biosensors, where aluminum thin films, polysilicon and SU8 are used as the beam for the cantilever [6], in this work a single-walled carbon nanotube (SWCNT) is used as the beam which offers a greater flexibility for the surface functionalization as well as more flexible mechanical properties. It is rather simple and more reliable to functionalize the SWCNTs surface through passive adsorption and covalent immobilization. The surface of the CNT beam is coated with gold nanoparticles and specific antibodies are physically immobilized on top of the CNT beam where antigens are specifically adsorbed on the antibodies. And, a molecular layer is used to protect the sensor against any unspecific adsorption.

In this paper, modeling and simulation of the mechanical deformation of a SWCNT beam and the associated mass change due to biological particle detection are described. We have used the FEM for the 3D coupled analysis of electrostatic field and the associated deformation of the beam. Two approaches are investigated for detection of biological activity on the CNT surface: (i) release of charge on the CNT surface and (ii) attachment of a mass.

II. ELECTROSTATICAL MODEL

Electrostatically driven nano-actuator is governed by coupled electrostatic and mechanical restoring forces. Thus, it is crucial to understand the relationship between the driving electrostatic force and the mechanical restoring force. In this design, an electrostatically actuated CNT beam is suspended above a stationary rigid substrate. Both structures are made of electrically conductive materials, and are separated by a dielectric medium (see Fig. 1). An initial voltage bias is applied between the two conductors generating an attractive electrostatic force between the two conductors. This force bends the beam toward the grounded layer below it. The addition of any ion released by biomolecular interactions of immobile and target molecules increases the force deforming the beam. Ideally, this is the design feature that is exploited to achieve biosensing.

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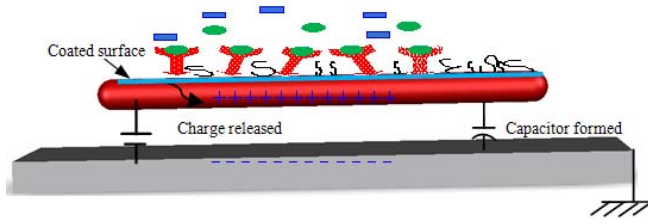


Fig. 1. A schematic drawing of an electrostatically driven CNT cantilever. A molecular layer (black) and receptor molecules (red) are attached to sensing layer.

Since the beam deforms due to the applied electrostatic forces, the electrostatic fields developed are further modified by the deformation. This is like a positive feedback between the electrostatic forces and the deformation of the cantilever beam. The deformation caused by the forces will reduce the gap to the grounded substrate. As a result of this reduction, the restoring force increases linearly, and at the same time the electrostatic force increases squarely. At a certain voltage, this leads to the phenomenon of pull-in. Determination of pull-in voltage is an important issue in the design process of nanosystems to quantify the sensitivity, instability and the dynamics of devices. To achieve the stable state, it is inherently necessary to develop an iterative algorithm. A flowchart for the electrostatic-mechanical coupled system is given in Fig. 2.

When an initial biasing voltage is applied between CNT and ground, a capacitance is formed. As long as the charge is increased on the beam surface by biomolecular interaction, the energy stored in the capacitor is increased by:

$$W = \frac{1}{2} \frac{Q(x)^2}{C} \quad (1)$$

where $Q(x)$ is the charge at a point x on the conductor surface. And the surface charge density on the conductor surface can be obtained as:

$$\rho(x) = -\epsilon \frac{\partial V(x)}{\partial x_i} n_i(x) \quad (2)$$

where $V(x)$ is the potential of the conductor, ϵ is the permittivity of the media and $n_i(x)$ is a vector whose direction is normal to inside of the conductor. The electrostatic field is derived from the following electrostatic equation:

$$-\nabla \cdot (\epsilon \nabla V(x)) = 0 \quad (3)$$

where derivatives are taken with respect to spatial coordinates. Next, the electrostatic force which causes the beam to bend can be found from the Coulomb's law:

$$\vec{F} = \frac{Q(x)^2}{4\pi\epsilon_0 r^2} \hat{r} \quad (4)$$

where $\hat{r}$ is the unit vector acting in the direction parallel to the line joining between the positive and negative charges. Finally, the force density per unit area is governed from the Maxwell's stress tensor:

$$\vec{F}_d = -\frac{1}{2} (\vec{E} \cdot \vec{D}) \vec{n} + (\vec{n} \cdot \vec{E}) \vec{D}^T \quad (5)$$

where, $\vec{E}$ and $\vec{D}$ are the electric field and electric flux density vectors respectively, and $\vec{n}$ is the outward normal vector of the boundary.

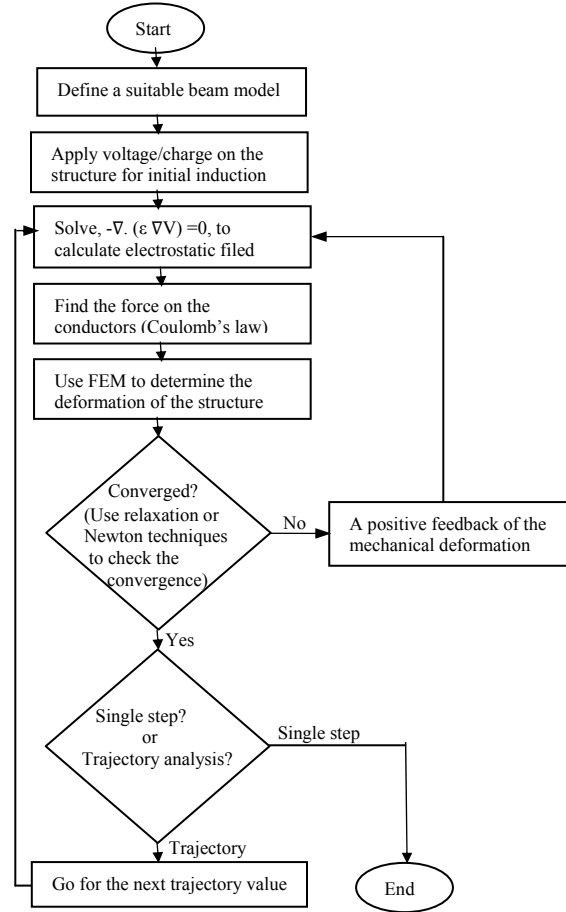


Fig. 2. A flowchart illustration of the algorithm for electrostatic-mechanical coupled analysis both for single step and trajectory.

III. MECHANICAL MODEL

In the mechanical analysis, the sensing measurement for the mass attached approach is considered in two ways: (i) change in the deflection of the beam, and (ii) resonant frequency shift. If a mass (mass of the biological object recognized by the receptor molecules) is attached to the free end of the SWCNT beam, it creates a stress to the surface which causes the beam to deflect. On the other hand, if the structure is an elastic body, then it becomes a harmonic oscillator which oscillates with the natural frequency. According to Hooks's law, the mechanical strain produced by this attached mass, m is:

$$\frac{\Delta Z}{Z} \propto \text{stress} \quad (6)$$

$$\text{but, stress} = \frac{F}{A} = \frac{mg}{A} \quad (7)$$

$$\text{so, } \frac{\Delta Z}{Z} \propto m \quad (8)$$

where $g=9.8\text{ms}^{-2}$, and A is the area affected by the stress.

From the well know calculus analysis, it has been shown that the defelection, d , of a cylindrical beam of radius R is:

$$d = \frac{mgL^3}{12\pi R^4 Y} \quad (9)$$

where Y is the Young's modulus and L is the length of the beam.

In the second approach, the resonance frequency of vibrating beam is expressed as:

$$f_0 = \frac{1}{2\pi} \sqrt{\frac{k}{m_{eff}}} \quad (10)$$

where, k is the elastic constant of the CNT $= \sqrt{\frac{3EI}{L^3}}$, m_{eff} is the effective mass for the oscillating CNT beam which relate to the real mass m [7] through $m_{eff} = 0.2429m$. The applied external mass loading will affect the resonant characteristics. The modified resonant frequency (f_{0m}) due to an extremely smaller mass loading (Δm_{eff}) is therefore,

$$f_{0m} = \frac{1}{2\pi} \sqrt{\frac{k}{m_{eff} + \Delta m_{eff}}} = f_0 \left(1 - \frac{1}{2} \frac{\Delta m}{m}\right) \quad (11)$$

$$\Delta f = f_{0m} - f_0 = -\frac{f_0}{2} \frac{\Delta m}{m} \quad (12)$$

Thus, the sensitivity for this small change of mass is therefore:

$$\text{Sensitivity} = \frac{\Delta f}{\Delta m} = \frac{f_0}{2m} \quad (13)$$

The effective mass, m_{eff} , of the CNT beam is $\frac{33}{140} \rho A L$ so, once Δf is known, one can easily find the value of the mass load on the beam from (11).

IV. THREE DIMENSIONAL FINITE ELEMENT ANALYSIS

In this study, the cylindrical CNT is modeled in 3-D using FEM software CoventorWare. A silicon substrate is used as the ground of the cantilevered biosensor which is $0.16 \mu\text{m}$ thick and coated with silicon nitride layer of $0.007 \mu\text{m}$. The geometry of the SWCNT used for the beam are as follows: outer diameter = 32 nm , wall thickness = 14.2 nm , length = $5.55 \mu\text{m}$, and located $0.045 \mu\text{m}$ above the ground. The surface of the CNT is coated with a thin layer of receptor molecule to produce the biological interaction on the surface. The substrate is meshed using the Manhattan parabolic mesh whereas, CNT is meshed using extruded bricks parabolic mesh due to its very high aspect ratio. In this modeling study, the sensing mechanism is studied in the following two platforms.

A. Electrostatical

As described above, an initial voltage bias is applied between the two conductors generating an attractive electrostatic force between the two conductors. Fig. 3 shows a contour plot for the initial addition of charge of $7.32 \times 10^{-4} \text{ pC}$. In Fig. 4, we have shown that the deformation of the beam increases as the additional charge is produced in the

CNT beam by the biological interaction with the receptor molecule. By using the cosolve solver with parametric set up with charge being the variable, it is shown that the beam deflects toward the ground until the pull-in. We have also shown that the variation of the beam's initial position affects the electrostatic force acting on the CNT beam as well as the capacitance formed (Fig. 5).

B. Mechanical

In the mechanical model, an equivalent mass for the corresponding target molecule is attached on the coated CNT surface. It is shown that, as the attached mass increases, the beam deflects more toward the ground substrate as illustrated in Fig. 6. Using the parametric solver, a trajectory variable is assigned to vary the attached mass from $0.0564 \mu\text{g}$ to $1.184 \mu\text{g}$.

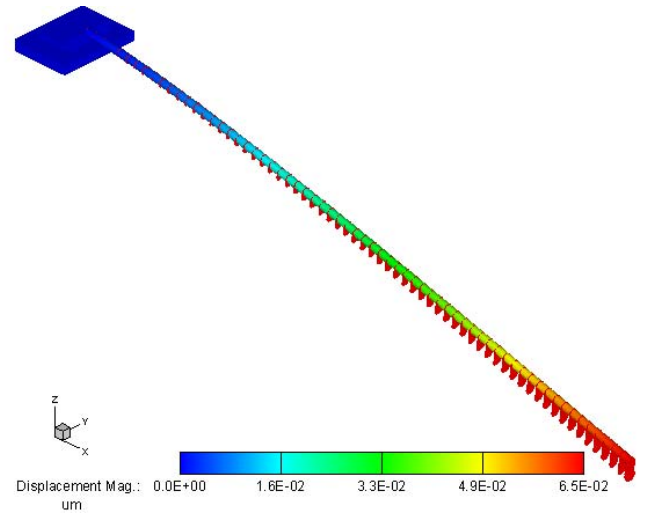


Fig.3. Contour plot of the coupled electrostatic-mechanic solver. Arrows indicate the direction of beam displacement.

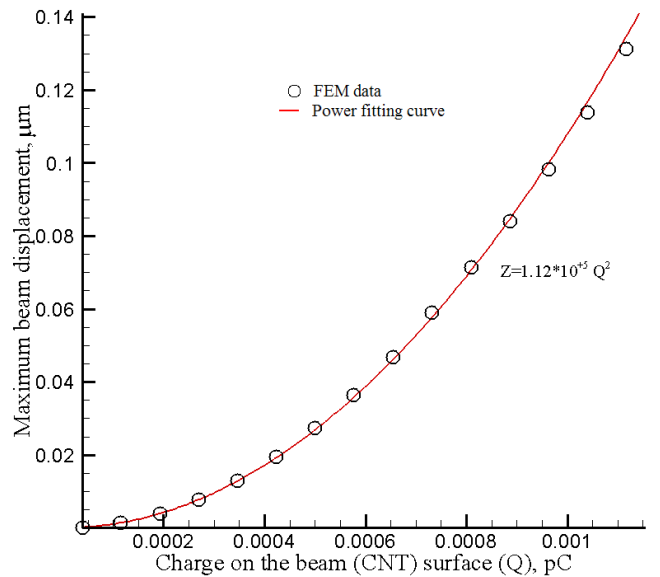


Fig. 4. Graph showing the relationship between the maximum displacement of the beam and the charge applied.

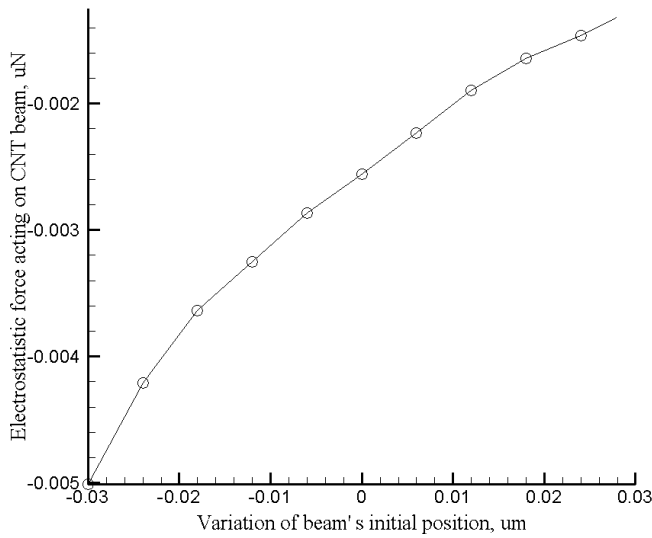


Fig. 5. Variation of the beam's position above and under its initial position to observe exert electrostatic force. A zero value in the plot indicates the beam's initial position (beam is $0.045\mu\text{m}$ above the ground) while the negative values denote beam being below its initial position.

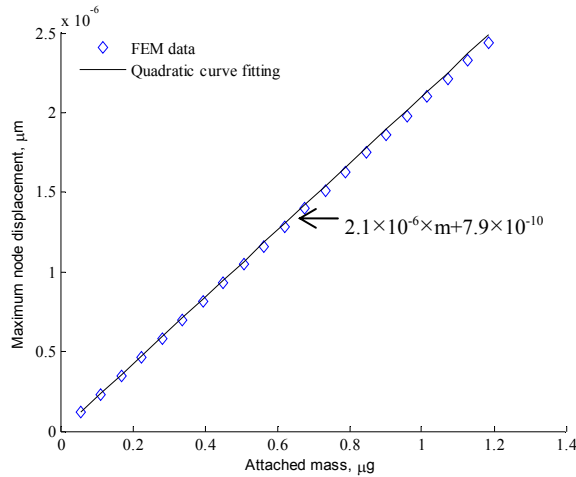


Fig. 6. Graph showing the relationship between the maximum displacement of the beam and the attached mass.

V. RESULTS AND DISCUSSIONS

To determine the electrical and mechanical response of the CNT cantilever biosensor, an additional charge or a mass is attached which is the result of any biological objects present on the CNT surface. In each case of the FEM simulation, an excellent agreement between the FEM acquired data and the mathematically developed theory has been achieved. It is shown that the displacement of the beam for these two approaches is best described by the following two equations:

$$Z_{\max} = 1.12 \times 10^5 Q^2, \text{ before pull-in} \quad (14)$$

and,

$$Z_{\max} = 2.1 \times 10^{-6} m + 7.9 \times 10^{-10}, \text{ before pull-in} \quad (15)$$

where, $Z_{\max}$ is the maximum beam deformation in μm , Q is the charge in pC, and m is the mass in μg . The maximum

beam displacement is linearly dependent with the mass attached which is in agreement of Hook's law (8). Whereas, it is directly proportional to the square of applied charge. It can be concluded that the electrostatic force is also directly proportional to the square of applied charge (as the electrostatic force is inversely proportional to the square of the distance between the conductors) which is in agreement with the Coulomb's law (4).

The sensitivity of this biosensor as a whole depends on a number of factors (e.g., length and diameter of CNT, position of beam and target probe). It is outlined in the earlier discussions by Li et al. [8] that the smaller diameter and larger length of CNT offer the enhanced sensitivity. In this study, however, we have investigated the variation of beam's position that also enhanced the sensitivity. Fig. 5 suggests that, as the beam tends to get closer to the ground substrate, the force acting on the beam increases which is almost inversely dependent to the square of the distance. To get the increased sensitivity, the beam should be made as close as possible to the ground substrate maintaining the pull-in condition.

VI. CONCLUSIONS

This study has developed a computationally efficient method for the SWCNT cantilever biosensor using CoventorWare. CNT is modeled by continuum based approach. Both the vibration behavior and the electrostatic behavior have been discussed. The presented results demonstrate that the proposed FEM model can provide a better understanding of the mechanical as well as the electrostatic-mechanical coupled behavior of CNTs and their applications in biosensing. Additionally, as CNT has a very high aspect ratio, it is much easier to make large distortion of the C-C bonds and thus, improved sensitivity.

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