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Investigations on Single-walled CNT based Bio-sensor Using Finite Difference Method

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Abstract **-** In the present study, a Nano mechanical resonator is designed and used for the process of virus detection. The biosensor is designed using the single-walled carbon nano-tube (SWCNT). The investigations are done on the vibrations of the cantilevered sensor, when the virus is present at the tip. The cantilevered SWCNT will be able to identify the virus that may be present at the tip of the resonator. The calculations for determining the natural frequency are done using the finite difference method. It is found that the designed sensor is able to provide measureable frequencies even when a light virus approaches the cantilever. The sensitivity of the entire system is found to be able to detect the virus in the zeptogram scale.

Keywords**:** NEMS, Biosensor, Viruses, SWCNT

1. Introduction

Nano Electro Mechanical Systems (NEMS) technology has gained a significant interest in medical and environmental diagnostics due to its potential performance and cost advantages. The developed NEMS can detect small concentration of target molecules (viruses) and have better sensitivity than conventional biosensors. Carbon nanotubes (CNT) and Boron nitride nanotubes (BNNT) are the promising candidates for such kind of diagnostics because of their unique electronic structure and properties, as previously shown (Wan et al., 1997). CNTs are highly stable in terms of thermal and chemical exposure. These properties along with their mechanical properties and thermal conductivity make CNTs a promising candidate for biosensors. In addition CNT has a very high aspect ratio, it is therefore much easier to make large distortion of carbon bonds, which in turn gives large elongation of the nanowire to have better sensitivity.

2. CNT as a Cantilever

A cantilever can be used to measure minute deformations due to surface stress, heat flow, differential expansion, charge release, mechanical, electrical or magnetic forces, as shown by Misiacos et al. (2009). Surface stress offers a means to deflections facilitating the measurement of physical or biochemical interactions because adsorption or binding applies expanding intramolecular forces on the coated surface causing to bend the cantilever. Even due to chemical, physical or environmental factors it produces the deflection in nanometer scale. However, depending on the mechanical properties of the device, the sensing (capacitance, piezoresistance or resonance frequency) principle varies. Also based on the parameters used for measuring the change, it can be either cantilever bending or shifts in the resonance frequency. A cantilever can be used for pH sensing, DNA hybridization, gas sensing, liquid sensing and protein detection. Knowles et al. (2009) have designed a microcantilever for protein accumulation where the surface stress generated by the interaction between protein and the coated beam to detect protein. Li et al. (2008) have designed a cantilever array with receptor molecules to simultaneously detect cancer and cardiac markers.

CNT provides good performance in terms of deflection and chemical sensitivity. The sensitivity of the cantilever biosensor is greatly influenced by the proper surface functionalization, and the selectivity is achieved through immobilizing specific receptors on the top of the surface. Unlike other cantilever biosensors, where aluminum thin films, polysilicon and SU8 are used as the material for cantilever, here CNT beam offers greater flexibility for the surface functionalization and flexible mechanical properties, as previously shown (Nugaeva el al., 2005)

3. Vibrational Analysis

The aim of this study is to develop the sensor based on SWCNT so as to be able to identify the virus that may be attached at the tip of the nanotube. In order to perform the vibrational analysis of the system "SWCNT and virus," we need information about the masses of various viruses. Table 1 contains information about the masses of various viruses. The viruses can be analyzed as concentrated point mass when its mass m is much less than the mass M of the SWCNT for the stipulated length of the sensor, whereas the virus should be treated as heavy mass when m is either comparable to M or exceeds it. In this framework, as shown by Haener (1958) the characteristic equation for the constant cross section cantilever beam with an additional mass at its free ends is as follows:

$$\frac{1}{\cosh(\beta L)} + \cos(\beta L) = -\beta L \frac{m}{M}(\tanh(\beta L)\cos(\beta L) - \sin(\beta L)) + (\beta L)^3 \frac{I_G}{ML^2}(\tanh(\beta L)\cos(\beta L) + \sin(\beta L)) + (\beta L)^4 \frac{mI_G}{M^2L^2}\left(\frac{1}{\cosh(\beta L)} - \cos(\beta L)\right) \quad (1)$$

where, $\beta_n = \sqrt[4]{M\omega_n^2/LEI}$, EI is the stiffness in bending, M is the total mass of the beam, m is the additional mass, n is the number of waves in $4L$ for the cantilever beam, L is the length of the beam, I_G is the moment of inertia of the mass m, and n is the nth frequency in rad/s. Fig. 1 gives the pictorial representation of the SWCNT cantilever with the virus at the tip.

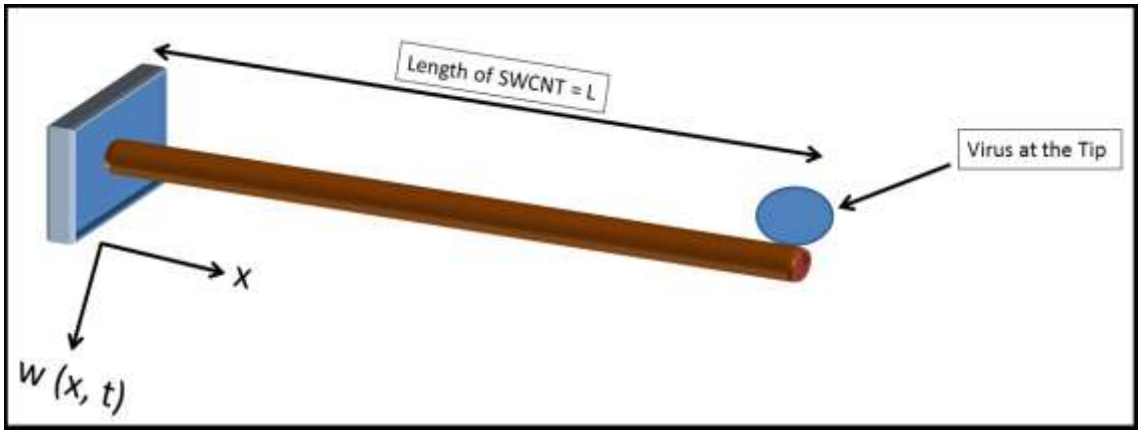

Fig. 1 SWCNT based cantilever with the virus at the tip.

Table. 1. List of some Viruses and their associated mass.

Sequel No.	Name of the Virus	Mass m_i (Da)
1.	Human Adenovirus Type 5	3.6×10^9
2.	Grouper Iridovirus	4.48×10^8
3.	Vaccinia Virus	1.72×10^8

Vibrational analysis of the SWCNTs with added virus depends on the ratio of the mass of the virus to that of the attached nanotube. Hereinafter, we will consider cases associated light virus.

The governing differential equations for free vibration of the SWCNTs read as

$$EI\frac{\partial^4 w(x,t)}{\partial x^4} + \rho A\frac{\partial^2 w(x,t)}{\partial t^2} = 0 \tag{2}$$

where, E is the modulus of elasticity, taken as 1 TPa, x is the axial coordinate, t is the time, w (x , t) is the transverse displacement, I is the moment of inertia, and A is the cross-sectional area of the nanotube. For the case $\mu \ll 1$, we can treat the virus as a concentrated mass. The boundary conditions for the fixed-free SWCNT with the light virus on the tip of the nanotube are

$$w(0) = 0, \qquad w'(0) = 0, \qquad w''(L) = 0, \qquad EI\frac{\partial^3 w(L,t)}{\partial x^3} - m\frac{\partial^2 w(L,t)}{\partial t^2} = 0 \tag{3}$$

where, L is the beam length. For the case when μ is of order unity or exceeds it, namely, when the mass attached to the beam tip is comparable with the mass of the SWCNT or is large in comparison to the beam's mass, one cannot treat the virus as a concentrated mass and neglect its rotary inertia. In particular, the boundary conditions, for the fixed-free SWCNT with the heavy virus at the end of the nanotube as shown by Soedel (1984), are

$$w(0) = 0, \qquad EI\frac{\partial^2 w(L,t)}{\partial x^2} + (I_G + ma^2) + ma\frac{\partial^2 w(L,t)}{\partial t^2} = 0$$

$$w'(0) = 0, \qquad EI\frac{\partial^3 w(L,t)}{\partial x^3} - m\frac{\partial^2 w(L,t)}{\partial t^2} - ma\frac{\partial^3 w(L,t)}{\partial t^2 \partial x} = 0 \tag{4}$$

where, I_G is the virus mass moment of inertia about its mass center and a denotes the distance between the virus center of mass and the tip of the beam.

4. Vibration Frequencies of SWCNT with Light Virus at the End of the Nanotube: Finite Difference Method

In this section, we use the finite difference method (FDM) to analyze the problem of vibration frequencies of a SWCNT with light virus at the end of the nanotube. We treat the virus as a concentrated mass ($\mu \ll 1$). The finite difference method proceeds by replacing the derivatives in the differential equations by finite difference approximations, as shown by Elishakoff et al. (2011). Instead of the differential equations, this procedure yields a system of algebraic equations that must be solved. The problem's domain is divided into a uniform grid of points or nodes spaced at distances equal to $h=L/N$, where N is the number of sections into which the beam of length L is divided. By using the central difference expression, the first and fourth derivatives of the displacement at a point j can be written as follows, respectively,

$$\frac{dw}{dx}(x_j) = \Delta^c w_j = \frac{w^{(j+1)} - w^{(j-1)}}{2h}$$

$$\frac{d^4w}{dx^4}(x_j) = \frac{1}{h^4}(w^{(j+2)} - 4w^{(j+1)} + 6w^{(j)} - 4w^{(j-1)} + w^{(j-2)}) \tag{5}$$

where, j is the number of the node with coordinate x_j, where the displacement is expressed. Equation (2) can be expressed at each node j as follows

$$\frac{EI}{h^4}(w^{(j+2)} - 4w^{(j+1)} + 6w^{(j)} - 4w^{(j-1)} + w^{(j-2)}) - \rho A w^2 w^{(j)} = 0 \tag{6}$$

Equation (6) is modified to the following form

$$(w^{(j+2)} - 4w^{(j+1)} + 6w^{(j)} - 4w^{(j-1)} + w^{(j-2)}) - \alpha w^{(j)} = 0 \tag{7}$$

where, the coefficient α is defined as

$$\alpha = \frac{\rho h^4 A \omega^2}{EI} \tag{8}$$

In order to find the vibration frequencies, we have to rewrite the boundary conditions specified by equation (3) in terms of central differences. In this circumstance, we obtain the following expressions:

$$w^{(0)} = 0, \qquad w^{(-1)} = w^{(1)}, \qquad w^{(N+1)} = 2w^{(N)} - w^{(N-1)},$$

$$w^{(N+2)} = 2w^{(N+1)} - 2w^{(N-1)} + w^{(N-2)} - \frac{2m\omega^2 h^3}{EI} w^{(N)} \tag{9}$$

Equation (7) must be satisfied at each nodal point j and it can be put in the matrix form

$$Aw = 0 \tag{10}$$

Where, A is an $N \times N$ matrix and $w = (w^{(1)}, w^{(2)}, \ldots, w^{(N)})^T$ is the nodal displacement vector. The determinant of matrix A must vanish in order to obtain the unknown roots ω_j. To illustrate the procedure we consider in detail the case when $N = 2$.

For $N = 2$ the boundary conditions defined by equation (9) leads to

$$w^{(0)} = 0, \quad w^{(-1)} = w^{(1)}, \quad w^{(3)} = 2w^{(2)} - w^{(1)}, \quad w^{(4)} = \left(4 - \frac{2m\omega^2 h^3}{EI}\right) w^{(2)} - 4w^{(1)} \tag{11}$$

By applying the boundary conditions equation (7) can be expressed in the matrix form as in equation (10) with

$$A = \begin{bmatrix} 6 - \alpha & -2 \\ -4 & 2 - \alpha - \dfrac{2m\omega^2 h^3}{EI} \end{bmatrix} \tag{12}$$

In order to have a nontrivial solution, the determinant of this matrix must be equal to zero, resulting in the frequency equation

$$r_0\omega^4 + r_1\omega^2 + r_2 = 0 \tag{13}$$

The values of the coefficients r_0, r_1 and r_2 is given as follows

$$r_0 = \frac{Ah^7\rho(2m + Ah\rho)}{E^2I^2}, \qquad r_1 = \frac{4h^3(3m + 2Ah\rho)}{EI}, \qquad r_2 = 4 \tag{14}$$

The solution of the fourth order polynomial equation (13) gives the desired natural frequencies. By increasing the number of segments that discretize the beam, the finite difference method will provide exact solution, as shown by Gaurav et al. (2014). Table 2 gives the specifications of the SWCNT and the results for ω_1 for various viruses are listed in Table 3.

Table 2. Specifications of the SWCNT

Density (g/m^3)	**Young's Modulus (TPa)**	**Length (μm)**	**Mass (g)**	**Inner Radius (R_i)(nm)**	**Outer Radius (R_o)(nm)**
2.3×10^6	1	5.55	9.544×10^{-18}	0.18	0.52

Table 3. Natural frequencies of SWCNT with the Virus at the end of the nanotube

Sequel No.	**Name of the Virus**	**Mass m_i (Da)**	**Finite Difference method (N=2) (Hz)**
1.	Human Adenovirus Type 5	3.6×10^9	3.67085×10^5
2.	Grouper Iridovirus	4.48×10^8	3.66702×10^5
3.	Vaccinia Virus	1.72×10^8	3.67084×10^5

5. Conclusion

In this paper we analyzed the detection of virus using a SWCNT. The natural frequency of the SWCNT has been calculated using the finite difference method, in the case when the virus is at the tip of the nanotube. Three viruses have been chosen in order to perform the study. The natural frequency is found to be increasing with the increase of the mass of the virus present at the tip of the nanotube. The frequency is found to be in the measureable range even when a very light virus is present. In future, this method can be used to detect viruses with very high precision and accuracy.

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