

## Research Article

# Computational Investigations of Fixed-Free and Fixed-Fixed Types Single-Wall Carbon Nanotube Mass Sensing Biosensor

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Using carbon nanotubes for sensing the mass in a biosensor is recently proven as an emerging technology in healthcare industry. This study investigates relative frequency shifts and sensitivity studies of various biological objects such as insulin hormone, immunoglobulin G (IgG), the most abundant type of antibody, and low-density lipoproteins (LDL) masses using the single-wall carbon nanotubes as a biomass sensor via continuum mechanics. Uniform distributed mass is applied to the single-wall carbon nanotube mass sensor. In this study, fixed-free and fixed-fixed type single-wall carbon nanotubes with various lengths of relative frequency shifts are studied. Additionally, the sensitivity analysis of fixed-free and fixed-fixed type CNT biological mass sensors is carried out. Moreover, node shapes studies are performed. The sensitivity results show better, if the length of the single-wall carbon nanotube is reduced.

## 1. Introduction

After discovering carbon nanotubes (CNT's) [1, 2], its utilization is found to be in diverse range of applications, such as nanomechanical resonators and nanobiological sensors. The unique great physical properties of the carbon nanotube lead to various usage in different fields such as nanoelectromechanical systems and actuators. [3–6]. The use of CNT in medical fields is enormous. Applications of CNT in electrochemical sensing [7–14], nanoactuators [15, 16], and nanosensors [5, 6, 17] are demonstrated. Nanomechanical resonators have been demonstrated in weigh cell, biomolecules, and gas molecules [18]. There is an increasing attention of CNTs in biological applications [5, 6, 19–21]. Difficulties of experimental and advantages of the theoretical modeling of nanoscale devices and CNTs are explained [3–5, 18, 22, 23].

By using CNT-based sensors, the sensing of volatile organic compounds related to human diseases is demonstrated [24], glucose oxidase (GOD) sensing using CNT is performed [25], and the extraordinary low detection limit of CNT working electrodes is shown [26]. Producing biosensors using CNT is an emerging trend. Many articles show the modeling techniques of elastic continuum mechanics concepts for analyzing the vibration of carbon nanotubes. The theory of the mechanical behaviors of materials dealing with continuous mass is called as continuum mechanics. There are two significances for the continuum modeling approach. It needs less work of the computational process than the molecular dynamics modeling, and nanostructures behavior analysis is much cheaper through the continuum model. Continuum beam and shell models have been elaborately studied. The beam theory concepts implemented using the single-wall carbon nanotube are explored [10]. The elastic

material properties and continuum models of carbon nanotubes have been studied [11].

The theory of mass recognition using CNT resonators is on the basis of the proven fact that the resonant frequency is sensitive to CNT resonator mass, which includes self-mass of the CNT resonator and attached mass. The change of attached mass on the CNT resonator triggers a change to the resonant frequency [27]. The sensitivity defined as the ratio of frequency shift to unit mass loaded is a linear function with the square of the mode number. Advantages of distributed mass load spanning the entire sensor surface in biological and chemical applications were discussed [28–30].

Innovations in microfabrication and nanofabrication technologies are permitting to attain significantly smaller mechanical transducers with micro-sized and nano-sized moving elements whose deformation and vibration are sensitively altered upon molecular adsorption. This type of mechanical biosensors is known as nanomechanical biosensors. The utilization of well-established semiconductor engineering allows the batch production of arrays of numerous nanomechanical systems. In general, all the nanomechanical biosensors are cantilever-shaped. So, developing the cantilever or bridge-type mechanical nanobiosensor is getting an important role in emerging medical industry.

In this study, we developed a computationally efficient single-wall carbon nanotube as a biological mass sensor with the continuum mechanics method using the finite element method. Using the biological objects such as insulin hormone, immunoglobulin G (IgG), and low-density lipoproteins (LDL) masses as a distributed load, the mass sensing investigations are carried out. In this study, fixed-free and fixed-fixed type single-wall carbon nanotubes with various lengths of relative frequency shifts and sensitivity analysis are examined. Additionally, the sensitivity analysis of fixed-free and fixed-fixed type CNT biological mass sensors is carried out.

## 2. Vibration Analysis of the CNT Model with Distributed Mass

Euler-Bernoulli theory is used to model SWCNT as resonators via continuum mechanics [31–33]. The motion of free vibration equation can be expressed as

$$EI \frac{\partial^4 u(x, t)}{\partial x^4} + \rho A \frac{\partial^4 u(x, t)}{\partial x^4} = 0, \quad (1)$$

where  $u(x, t)$ ,  $E$ ,  $I$ , and  $\rho$  are considered as the transverse deflection, Young's modulus, second moment of the cross-sectional area  $A$ , and the density of SWCNT, respectively. The fundamental frequency can be expressed as

$$f_n = \frac{1}{2\pi} \sqrt{\frac{k_{eq}}{m_{eq}}}, \quad (2)$$

where  $k_{eq}$  is the equivalent stiffness, and  $m_{eq}$  is the first mode vibration of attached mass with SWCNT mass. In this study, two different boundary constraints named as fixed-free and

fixed-fixed type is considered for the mass sensing analysis of the biosensor.

*2.1. Analysis of SWCNT with Fixed-Free Boundary Condition.* Figure 1 shows SWCNT with fixed-free boundary condition. By taking into account, the length  $L$  of SWCNT is perturbed with the uniform mass  $M$ , i.e., at  $x=L$ . The resonance frequencies of fixed-free SWCNT can be attained from

$$f_j = \frac{\lambda_j^2}{2\pi} \sqrt{\frac{EI}{\rho AL}}, \quad (3)$$

where  $\lambda_j$  values are acquired [34] and expressed the subsequent transcendental equation

$$\cos \lambda \cosh \lambda + 1 = 0. \quad (4)$$

The mode shapes of vibrations can be attained as

$$Y_j(\xi) = \left( \cosh \lambda_j \xi - \cos \lambda_j \xi \right) - \left( \frac{\sinh \lambda_j - \sin \lambda_j}{\cosh \lambda_j - \cos \lambda_j} \right) \cdot \left( \sinh \lambda_j \xi - \sin \lambda_j \xi \right), \quad (5)$$

where  $\xi = x/L$  is the length of CNTs along normalized coordinate. The first mode of vibration is significant for the sensing applications, and the value is  $\lambda_1 = 1.8751$  [35]. The value is attained by executing the transcendental (4).

$$k_{eq} = 12.36 \frac{EI}{L^3}; \quad (6)$$

$$m_{eq} = \rho AL + 4M.$$

Since we have applied distributed load where

$$M = m \times \gamma L, \quad (7)$$

$$f_n = \frac{1}{2\pi} \sqrt{\frac{k_{eq}}{m_{eq}}} = \frac{1}{2\pi} \frac{\alpha_k \beta}{\sqrt{1 + \alpha_m \Delta M}}, \quad (8)$$

where

$$\alpha_k = 3.5,$$

$$\alpha_m = 4,$$

$$\Delta M = \frac{M}{\rho AL}, \quad (9)$$

$$\beta = \sqrt{\frac{EI}{\rho AL^4}}.$$

*2.2. Analysis of SWCNT with Fixed-Fixed Boundary Condition.* For the fixed-fixed boundary condition shown in Figure 2, the motion and the natural frequency equations are followed by (1) and (2), respectively.

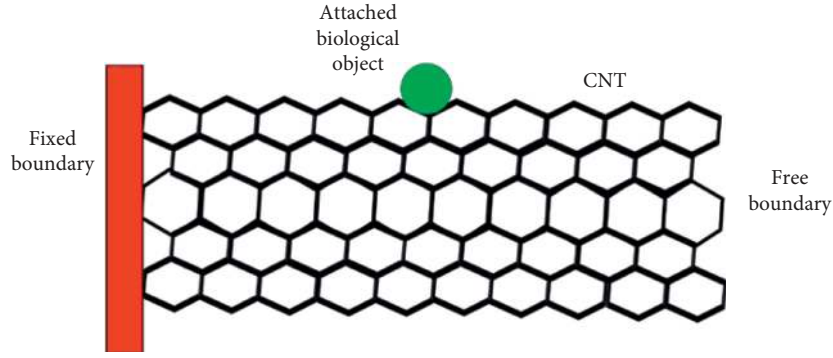


FIGURE 1: SWCNT with fixed-free boundary condition.

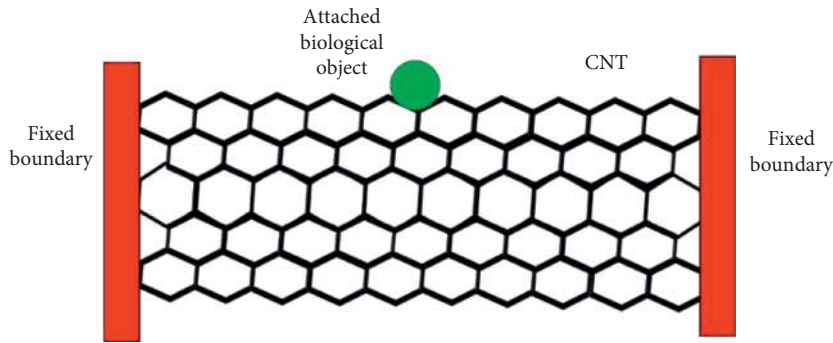


FIGURE 2: SWCNT with fixed-fixed boundary condition.

Moreover, the  $\lambda_j$  values are attained [34] by executing

$$\cos \lambda \cosh \lambda + 1 = 0. \quad (10)$$

The mode shape of vibration is stated as

$$Y_j(\xi) = (\cosh \lambda_j \xi - \cos \lambda_j \xi) - \left( \frac{\cosh \lambda_j - \cos \lambda_j}{\sinh \lambda_j - \sin \lambda_j} \right) (\sinh \lambda_j \xi - \sin \lambda_j \xi), \quad (11)$$

where  $\xi = x/L$ , and the value of first mode vibration is  $\lambda_1 = 4.7300$  [35]. Using equation (6), the mode shape normalizing is carried out.

$$k_{eq} = 500.56 \frac{EI}{L^3}; \quad (12)$$

$$m_{eq} = \rho AL + 2.52M.$$

Since we have applied distributed load and  $M = m \times \gamma L$ ,

$$f_n = \frac{1}{2\pi} \sqrt{\frac{k_{eq}}{m_{eq}}} = \frac{1}{2\pi} \frac{\alpha_k \beta}{\sqrt{1 + \alpha_m \Delta M}}, \quad (13)$$

where

$$\alpha_k = 22.37,$$

$$\alpha_m = 2.52,$$

$$\Delta M = \frac{M}{\rho AL}, \quad (14)$$

$$\beta = \sqrt{\frac{EI}{\rho AL^4}}.$$

**2.3. Analysis of Mass Detection.** For the free vibrations of CNT substituting  $M = 0$  in (8), the resonant frequency is attained as

$$f_{0n} = \frac{1}{2\pi} \alpha_k \beta. \quad (15)$$

From (13) and (15), the resonant frequency shift attained due to the distributed attached mass can be expressed as

$$\Delta f = f_{0n} - f_n = f_{0n} - \frac{f_{0n}}{\sqrt{1 + \alpha_m \Delta M}}, \quad (16)$$

and the added mass actual value can be attained as

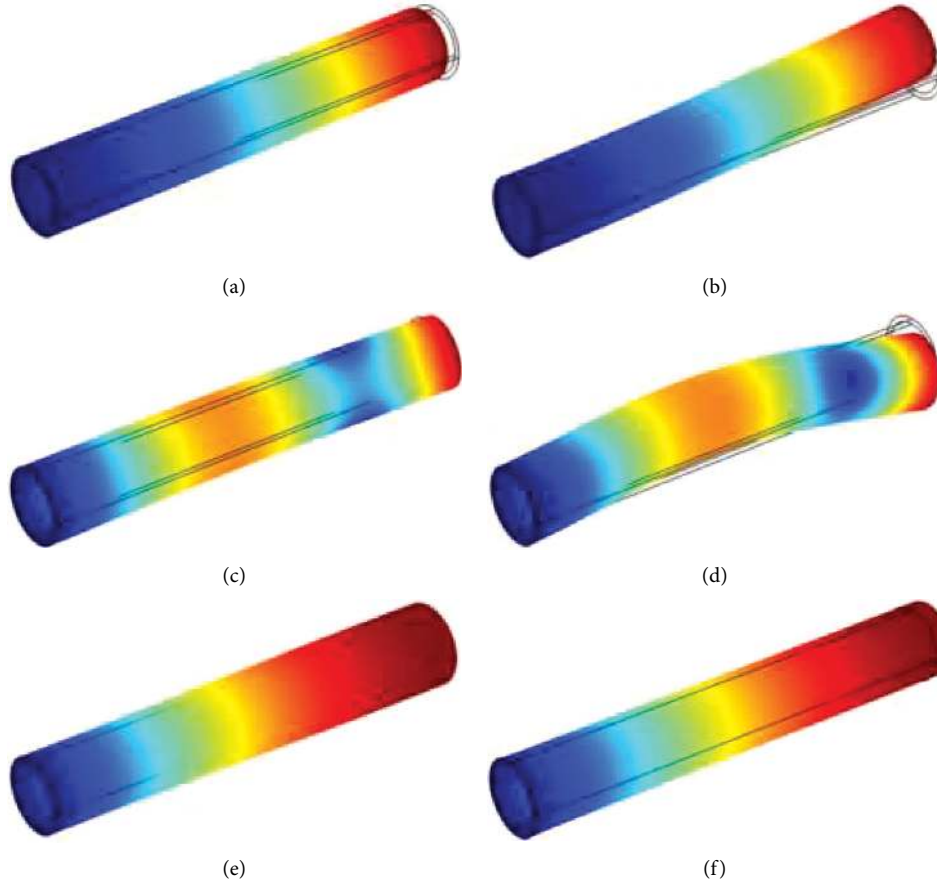


FIGURE 3: Fixed-free carbon nanotube fundamental frequency analysis for L/D ratio 7.2. (a) Fundamental frequencies F1, (b) F2, (c) F3, (d) F4, (e) F5, and (f) F6.

$$M = \frac{\rho AL}{\alpha_m} \frac{(\alpha_k^2 \rho^2)}{(\alpha_k \beta - 2\pi \Delta f)^2} - \frac{\rho AL}{\alpha_m}. \quad (17)$$

The (17) relates the added mass with the shift of frequency.

### 3. Model Validation

Figures 3 and 4 show the fixed-free and fixed-fixed based CNT models' mode shapes for 6 fundamental frequency levels for the length to diameter ratio 7.27 for getting the precision of our model. To find the accuracy of the present CNT model, initially, our finite element CNT model is verified with previous molecular dynamics and commercially available finite element model for the same material properties and the dimensions.

Figure 5 shows the fundamental frequency comparisons for the present FEM work with the existing work. The results are compared with the previous study and will be agreed with that study. The values of the existing work and present work are given in Table 1. From the table, it has been clearly demonstrated that our model CNT provides minimum discrepancy compared to the previous length to diameter ratio studies, and it provides the assurance to take on further

studies as a biological mass sensor. The value of  $E$  and  $\rho$  is taken as 1:0 TPa and 2:24 g/cc, respectively [53].

## 4. Results and Discussion

**4.1. Resonant Frequency Analysis for Fixed-Free Boundary.** The continuum mechanics single-wall CNT is modelled as fixed-free beam, where one end is to be fixed and other end is to be free. Figure 6 shows the fixed-free type CNT. Distributed load is uniformly applied on CNT. The fixed-free CNT is initially assumed straight and no extensile and loaded the distributed forces uniformly. From this technique, the mechanical behavior of the nanoresonator biosensor solutions provided is accurate and reliable. Using this system, the mode shapes analysis and frequency shift studies of the nanobiosensor are performed. Figure 7(a) shows SWCNT from fundamental frequency to six changes of frequencies without attaching any mass on CNT. In the fixed-free mode, the length of the carbon nanotube is changed from 2 nm to 20 nm to obtain the various results and mode shapes analysis up to 6 levels. The diameter of the carbon nanotube is 1.1 nm for all the studies in this work. The change of frequencies is in GHz. To understand SWCNT as a nanobiomass sensor, in this study, three

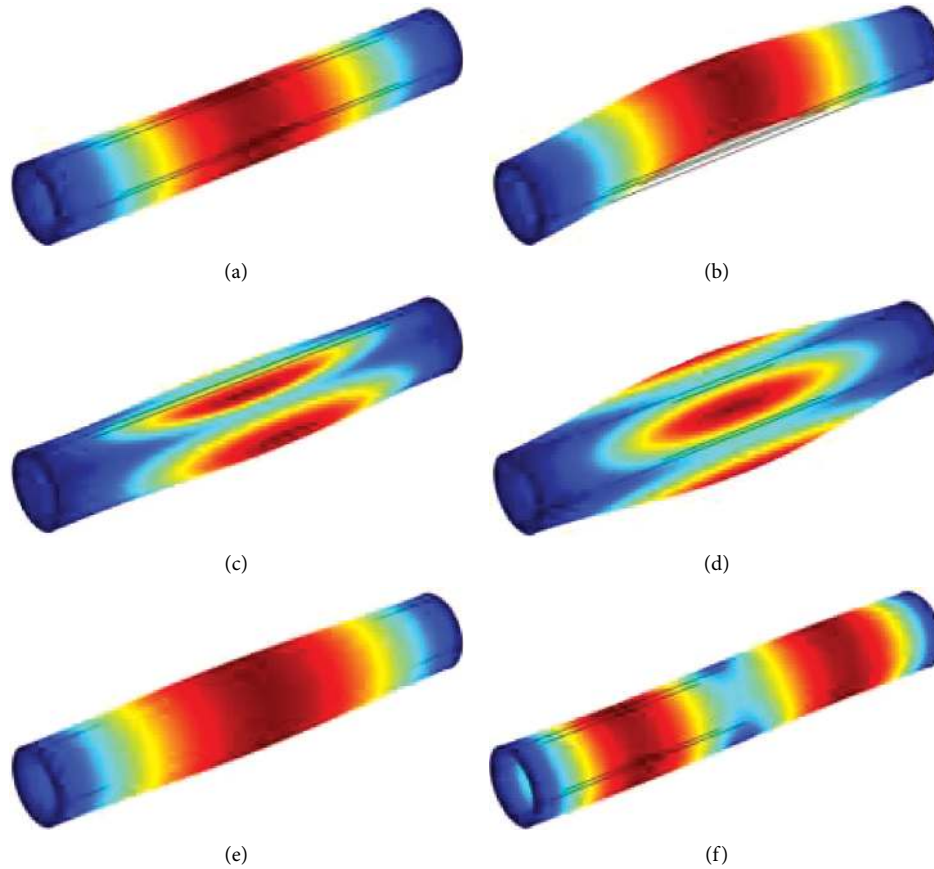


FIGURE 4: Fixed-fixed carbon nanotube fundamental frequency analysis for L/D ratio 7.2. (a) Fundamental frequencies F1, (b) F2, (c) F3, (d) F4, (e) F5, and (f) F6.

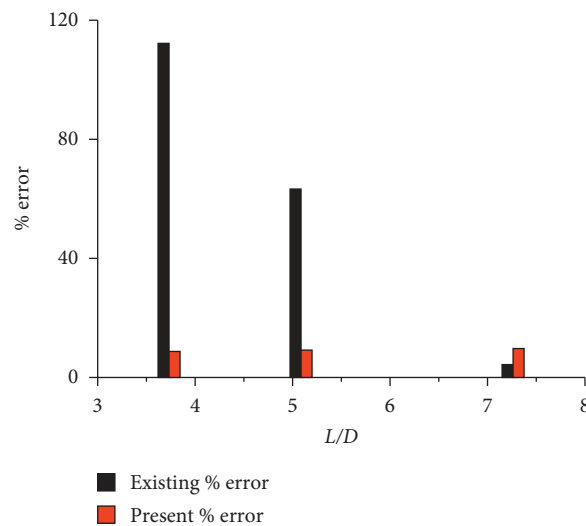


FIGURE 5: Fundamental frequency comparisons for the present FEM work with existing works.

biological objects insulin hormone, immunoglobulin G (IgG), the most abundant type of antibody, and low-density lipoproteins (LDL) masses are considered. The mass values

of insulin hormone 9.644 zg, immunoglobulin G 249.081 zg, and low-density lipoproteins 4981.620 zg are taken into account for the analysis. Compared to different

TABLE 1: Fundamental frequency comparisons for the present FE work with existing MD work.

<i>L/D</i>	Fundamental frequencies	MD [17]	FE [27]	% error	Present	% error
3.727	F1	10.315	10.769	-4.40	<b>9.409</b>	<b>-8.78</b>
	F2	10.315	10.769	-4.40	<b>9.411</b>	<b>-8.75</b>
	F3	10.478	16.859	-60.90	<b>9.945</b>	<b>-5.08</b>
	F4	10.478	22.224	-112.10	<b>9.946</b>	<b>-5.07</b>
	F5	15.796	22.224	-40.69	<b>14.589</b>	<b>-7.63</b>
5.090	F1	6.616	6.683	-4.04	<b>6.561</b>	<b>-0.82</b>
	F2	6.616	6.884	-4.05	<b>6.561</b>	<b>-0.82</b>
	F3	9.143	12.237	-33.84	<b>8.329</b>	<b>-8.89</b>
	F4	9.143	14.922	-63.21	<b>8.333</b>	<b>-8.85</b>
	F5	11.763	14.924	-26.87	<b>10.986</b>	<b>-6.60</b>
7.272	F1	3.800	3.900	-2.63	<b>3.845</b>	<b>1.19</b>
	F2	3.800	3.900	-2.63	<b>3.845</b>	<b>1.20</b>
	F3	8.679	8.659	-0.23	<b>7.840</b>	<b>-9.65</b>
	F4	8.679	9.034	-4.09	<b>7.844</b>	<b>-9.61</b>
	F5	8.801	9.034	-2.65	<b>8.189</b>	<b>-6.94</b>

Present work provided better error results than previous works.

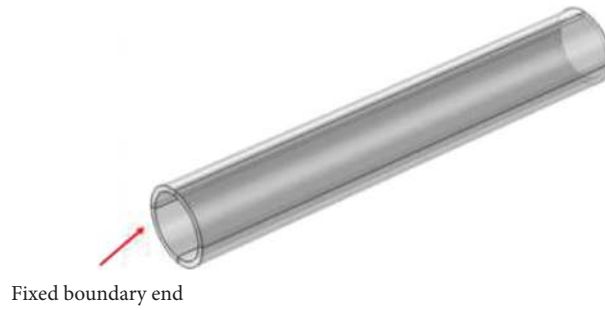


FIGURE 6: Fixed-free boundary fundamental frequency analysis (one end is fixed and another one end is free).

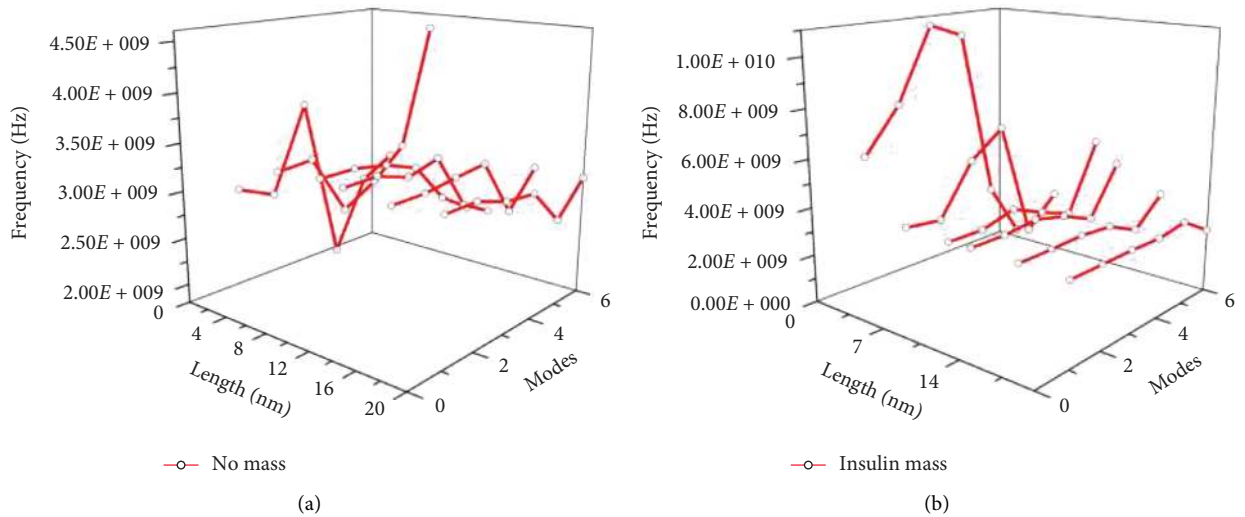


FIGURE 7: Continued.



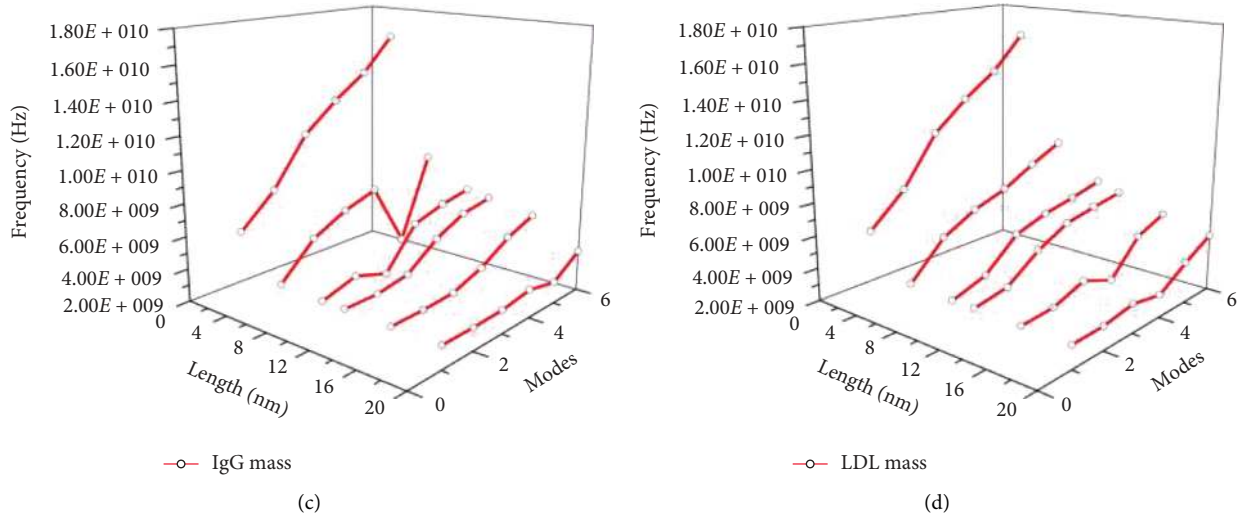


FIGURE 7: (a) Fixed-free boundary fundamental frequency for CNT with no mass and frequency shift analysis for (b) insulin, (c) IgG, and (d) LDL biological objects mass attached.



FIGURE 8: Fixed-fixed boundary fundamental frequency analysis (both the ends are fixed).

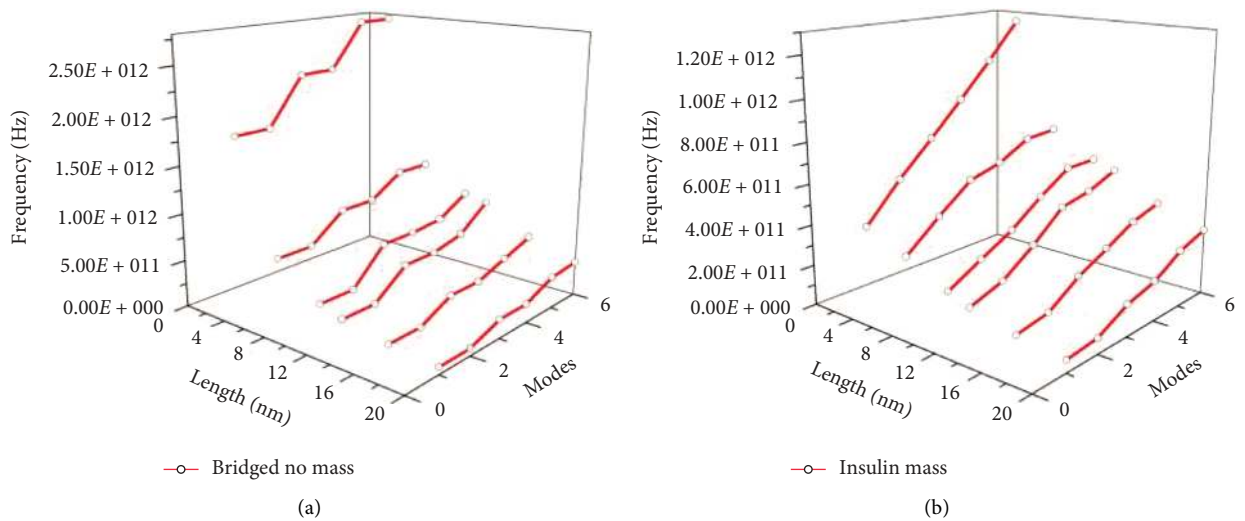


FIGURE 9: Continued.

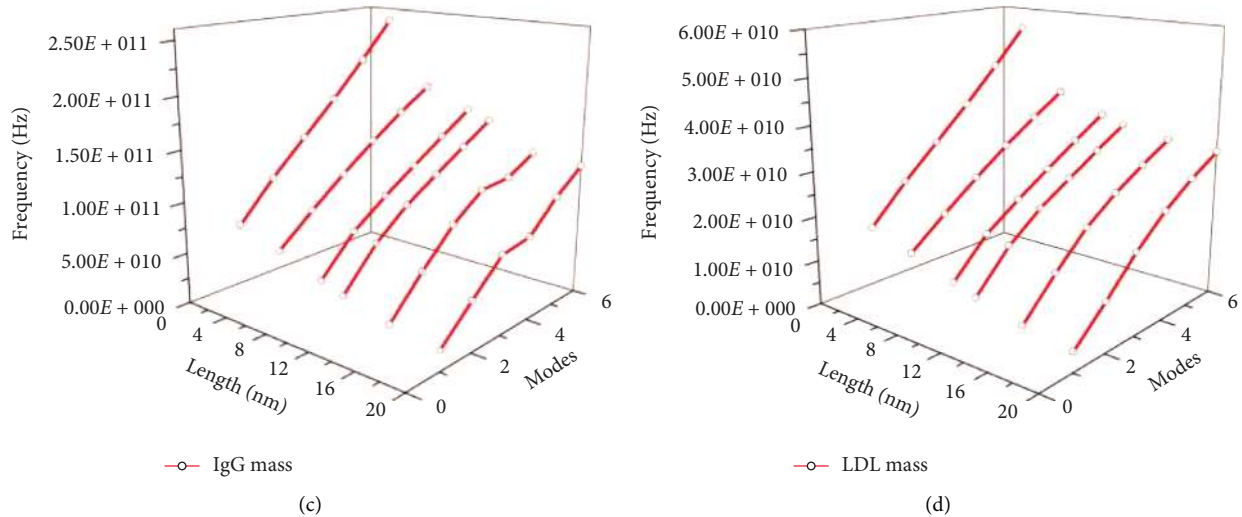


FIGURE 9: (a) Fixed-fixed boundary fundamental frequency for CNT with no mass and frequency shift analysis for (b) insulin, (c) IgG, and (d) LDL biological objects mass attached.

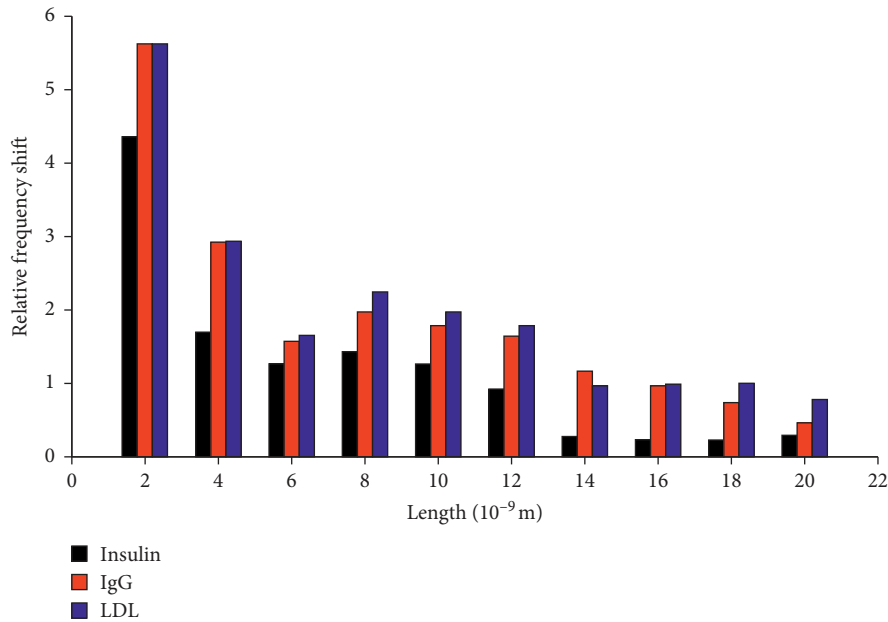


FIGURE 10: Comparisons of fixed-free boundary relative frequency shift analysis for CNT.

distributed uniform masses attached with fixed-free SWCNT, the frequency changes occurred reasonably. The mode shape and frequency shift changes are shown in Figures 7(b)–7(d). From the results, it can be understood that the lower dimensions CNT highly varied rather than higher dimensions CNT.

#### 4.2. Resonant Frequency Analysis for Fixed-Fixed Boundary.

Both the boundary ends of SWCNT is fixed and is investigated with the no mass and with the added mass of insulin hormone, immunoglobulin G, and low-density lipoproteins independently for the various length of CNT. While adding mass on the bridge-type SWCNT, mode shapes variations are very high. Figure 8 shows the

fixed-fixed type CNT. Figures 9(a)–9(d) show SWCNT resonant frequency with no mass and the insulin hormone, immunoglobulin G, (IgG), and low-density lipoproteins (LDL) masses.

From the results, compared to no mass CNT resonant frequency and the insulin hormone, IgG, and LDL masses, it can be understood that when the mass of objects increases, the resonant frequency of CNT reduces. The higher mass of the low-density lipoproteins (LDL) resonant frequency is lower than others.

#### 4.3. Comparisons of Relative Frequency Shift Analysis for Fixed-Free and Fixed-Fixed Type CNT.

To identify various biomasses sensing for different biological objects, the



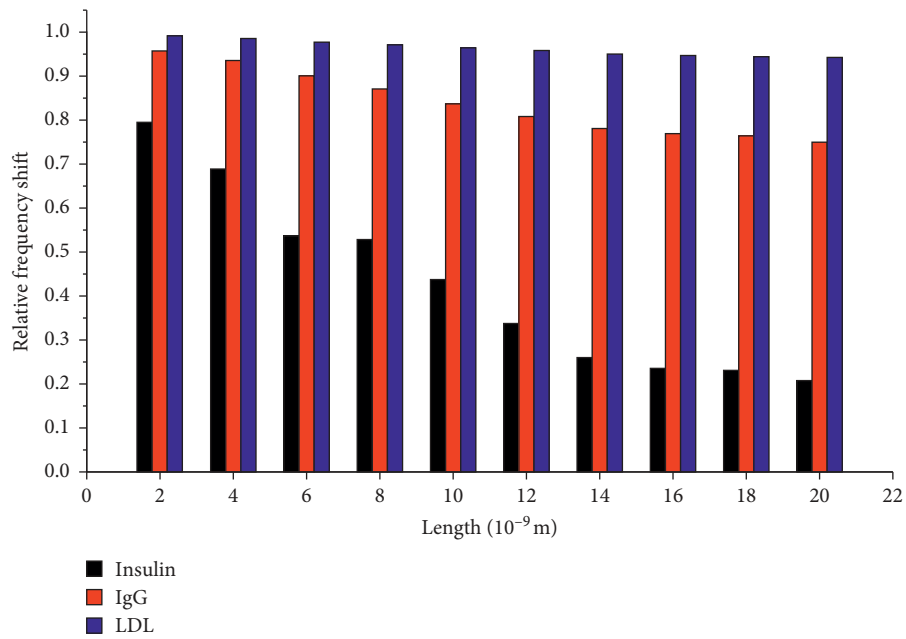
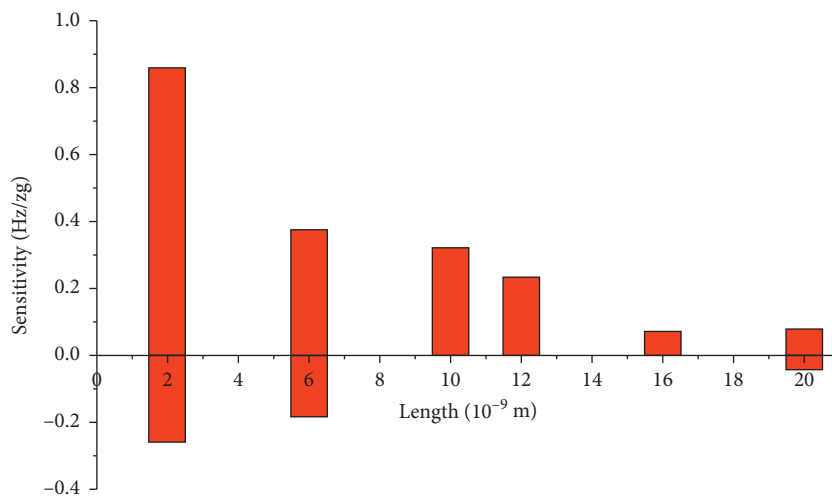


FIGURE 11: Comparisons of fixed-fixed boundary relative frequency shift analysis for CNT.



(a)

FIGURE 12: Continued.

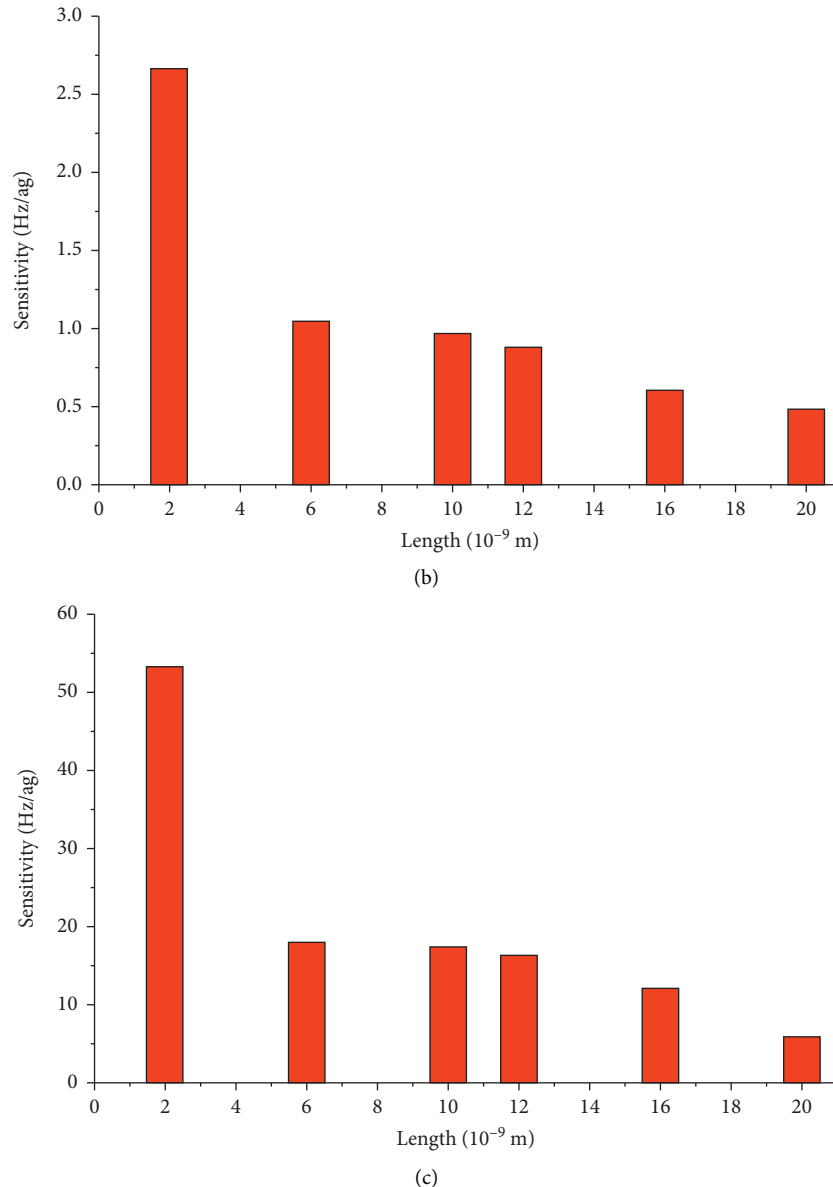


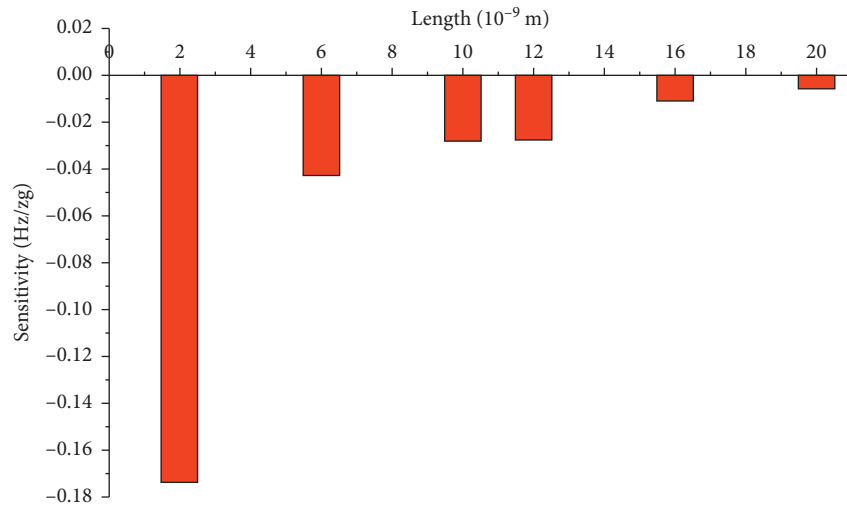
FIGURE 12: Fixed-free boundary sensitivity analysis for (a) insulin, (b) IgG, and (c) LDL biological objects mass attached.

frequency shift studies are carried out for fixed-free and fixed-fixed SWCNT. Figure 10 shows the frequency shift results of the insulin, IgG, and LDL biological sensing output on fixed-free SWCNT. Figure 10 shows that when the length of the CNT is reduced, the frequency shift is increased. But the length of CNT 6–12 nm provides better variation frequency shift for biosensing.

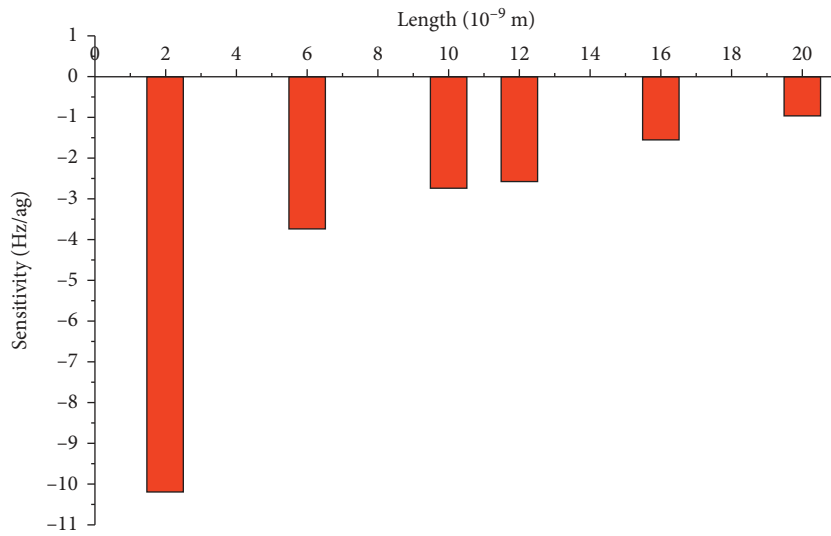
Figure 11 shows the results of the fixed-fixed type SWCNT frequency shift for various biological objects. Since both the ends are fixed, the relative frequency shift results show the clear difference between all the length of CNTs and insulin, IgG, and LDL mass sensing. Reducing the length of the CNT provides higher shifts rather than higher length CNTs.

**4.4. Sensitivity Analysis for Fixed-Free and Fixed-Fixed Type CNT.** To investigate the accuracy of biomass sensing for different biological objects, the sensitivity studies are important. Figures 12(a)–12(c) show insulin, IgG, and LDL sensing for the fixed-free CNT. Based on the mass of the insulin, IgG, and LDL, the sensitivity level has been varied, and it can be clearly identified. The sensitivity level gets high, when the length of CNT is reduced. When adding the low mass of insulin, the zeptogram level sensitivity is achieved, and when the mass increased for IgG and LDL, attogram sensitivity is attained.

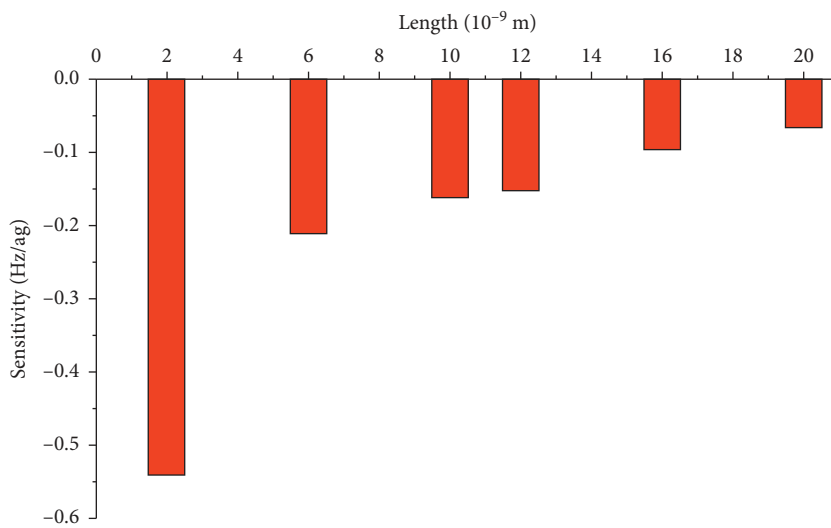
Figures 13(a)–13(c) show insulin, IgG, and LDL sensing for the fixed-fixed CNT. Insulin sensitivity is lower than IgG



(a)



(b)



(c)

FIGURE 13: Fixed-fixed boundary sensitivity analysis for (a) insulin, (b) IgG, and (c) LDL biological objects mass attached.

and LDL. Compared to the fixed-free type, the sensitivity is reduced in the fixed-fixed type CNT.

## 5. Conclusion

Biological sensing with the one-dimensional nanostructure is one of the vital roles in clinical and healthcare industries. In this study, we have modelled computationally efficient single-wall carbon nanotube as a biological mass sensor with the continuum mechanics technique using a finite element numerical package. The investigations are carried out using the resonant frequency analysis method. To prove the accuracy of the model, the SWCNT model is tested with the previous study [27]. Insulin hormone, immunoglobulin G (IgG), and low-density lipoproteins (LDL) masses are considered for analyzing as a biological mass sensor. In this study, fixed-free and fixed-fixed type single-wall carbon nanotubes with various lengths of relative frequency shifts are studied for insulin, IgG, and LDL. Additionally, the sensitivity analysis of fixed-free and fixed-fixed type CNT biological mass sensor is carried out. This study clearly shows that the change of biological object masses will change the frequency shift and the sensitivity of the SWCNT sensor. From the outcomes, it can be understood that SWCNT can be employed as a high-accuracy biological mass sensor for various biological objects when reducing the length of CNTs. While attaching the biological objects in the CNT nanobiosensor, the complications in measuring high number of vibration modes and loss of mechanical energy in liquids have to be explored in future.

## Data Availability

The data used to support the findings of this study are included within the article.

## Conflicts of Interest

The authors declare that they have no conflicts of interest.

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