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Procedia Materials Science 5 (2014) 2 – 10

Procedia Materials Science

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International Conference on Advances in Manufacturing and Materials Engineering,
AMME 2014

Continuum Solid Modeling Based FEM Simulation Approach For Single Walled Boron Nitride Nanotube Based Biosensing

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Abstract

The present paper investigates the vibrational characteristic of fixed free single walled boron nitride nanotube with attached bacterium or virus on free end to explore their suitability as bacterium or virus detector device or biosensor. The continuum solid modeling based finite element method approach has been used to analyze the various modes and resonant frequency shift caused by bacterium or virus on beam tip. The obtained simulation results have been compared with analytical results based on fixed free beam bending model. To be more precise in present analysis, the vibrational characteristic of four types of single walled boron nitride nanotubes of different lengths of same diameter have been considered. The different types of bacterium or virus at the tip of the fixed free single walled boron nitride nanotubes have been analyzed for their resonant frequency variation based analysis. The obtained simulation results have been found in sensible agreement with the analytical results. The obtained simulation results suggest that detection of the bacterium or virus having mass of 2.90 x 10^{-23} kg can be effectively performed.

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*Keywords:*Boron nitride nanotube, Continuum solid modeling, FEM, Biosensing.

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1. Main text

Boron nitride nanotubes (BNNTs) were theoretically predicted in 1994 [Rubio et al. (1994)] followed by their eminent fabrication by arc discharge in 1995 [Chopra et al. (1995)]. Potential of BNNTs in nanoscale devices lies in-

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Selection and peer-review under responsibility of Organizing Committee of AMME 2014
doi:10.1016/j.mspro.2014.07.236

fact that compared to carbon nanotubes (CNTs), they possess higher mechanical properties, thermal stability, electrical insulation and oxidation resistance at higher temperature in atmosphere [Li et al. (2008) and Moon et al. (2004)]. BNNTs are extremely thin tubes whose diameter is order of few nanometers, however whose length may be many times larger. As a structural analogue of CNTs in nature, in BNNTs alternating B and N atoms entirely substitute for C atoms with nearly no modification in atomic spacing [Oberlin et al. (1976) and Iijima (1991)]. In fact BNNTs are the robust light weight nanomaterials with a young's modulus of 1.2 TPa [Krishnan et al. (1998) and Chopra et al. (1998)]. In recent years, biosensors have been increasingly demanded in biological studies, health science research, drug delivery and clinical diagnosis [D'Orazio (2011), Tothill (2009) and Justino et al. (2010)]. Mass detection of biomolecules is recognized as key technology for predictive and preventive medicine. Prediction of disease is based on sensing the corresponding biomolecules. Ciofani et al. (2009) had explored the use of BNNTs in nanomedicine field and concluded that because of chemical stability of BNNTs, they are more stable for development of biosensing devices. Further Ciofani et al. (2010) reported that BNNTs have potential for future experiments to investigate their use as nano materials for accurate assessment of their bio compatibility. The principle of nano mechanical biosensor is based on the fact that resonant frequency is incredibly sensitive to mass of the added/attached biomolecule to the sensor system. The variation of added/attached mass in terms of different types of biomolecule to sensor system causes shift to the resonant frequency. Key issue of mass detection is in quantifying the shift in resonant frequency because of mass of connected biomolecule.

In the present work, the feasibility of single walled boron nitride nanotube (SWBNNT) as biosensor has been explored considering the possible adsorptions of various bacterium or viruses at the tip of the fixed free configuration of nanotube. The continuum solid modeling based finite element method (FEM) approach has been used to analyze the resonant behavior of fixed free SWBNNT with added nanoscale mass of the different bacterium/viruses at the tip. The SWBNNTs of length 2 μm, 1.5 μm, 1 μm and 0.5 μm are considered for the present analysis. Based on the fact that variation of nanotube diameter does not play significant role in change in resonant frequency and smaller the nano mechanical mass sensor more sensitivity it owns [Panchal et al. (2012a)]. The diameter of each considered SWBNNT is taken as 2 nm. For the transmission of the stresses on application of external load, the equilibrium between the continuum solid model and real atomistic model of the nanotube can be maintain by considering the effective thickness of the SWBNNT as 0.065 nm [Panchal et al. (2012a, 2012b)]. The bending vibration modeling of the fixed free SWBNNT has been performed and obtained analytical results have been used to validate the continuum solid modeling based simulation results. The various masses of the different considered bacterium/viruses have been quantified with respect to change in resonant frequency shift, to assure the feasibility of SWBNNT based biosensor system.

2. Bending vibration modeling of fixed-free beam

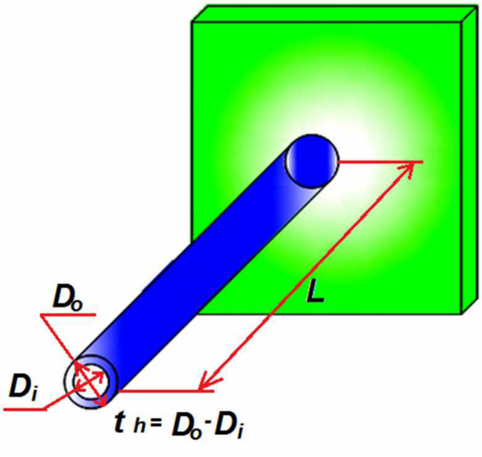

Fig. 1. Fixed free SWBNNT based sensor system of length L.

Boundary conditions:
At fixed end,

$$w(0,t)=0 \text{ and } \frac{dw}{dx}=0$$

At free end,

$$EI\frac{d^2w}{dx^2}=0 \text{ and } EI\frac{d^3w}{dx^3}=0$$

Equations of motion considering Euler beam model can be given as [Rao (1995)],

$$\rho A\frac{\partial^2 w}{\partial t^2}+EI\frac{\partial^4 w}{\partial x^4}=0 \tag{1}$$

The transverse displacement can be given as,

$$w(x,t)=e^{iwt}W(x) \tag{2}$$

The eigen value problem can be obtained as,

$$-\omega^2 W \rho A + EI\frac{d^4W}{dx^4}=0 \tag{3}$$

The general solution to this problem is given as,

$$W(x)=\beta_1\cosh x+\beta_2\sinh\beta x+\beta_3\cos\beta x+\beta_4\sin\beta x \tag{4}$$

Applying boundary condition to above eq. (4)

i.e. $W(0)=0;\left.\frac{dW}{dx}\right|_{x=0}=0;\left.\frac{d^2W}{dx^2}\right|_{x=1}=0;\left.\frac{d^3W}{dx^3}\right|_{x=1}=0$ and putting in matrix form we have,

$$\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ \cosh\beta l & \sinh\beta l & -\cos\beta l & \cosh\beta l \\ \sinh\beta l & \cosh\beta l & \sin\beta l & -\cosh\beta l \end{bmatrix}\begin{Bmatrix}\beta_1\\ \beta_2\\ \beta_3\\ \beta_4\end{Bmatrix}=0 \tag{5}$$

For non trivial solution determinant should vanish which gives characteristic equation for fixed free beam as

$$\cos\beta l\cosh\beta l+1=0 \tag{6}$$

For higher modes,

$$\cos\beta l=0 \tag{7}$$

Hence, solving eq. (6),

$$\beta_n l=\left(\left(\frac{2n-1}{2}\right)\pi+e_n\right) \tag{8}$$

Where n=1, 2, 3… and en is error by which βnl deviates for cosβl = 0

By calculating numerically, for first mode e1 = 0.3042, for second mode e2 = - 0.018 and for third mode e3 = 0.001.

From eq. (8)

$$\beta^2{}_n=\left(\left(\frac{2n-1}{2}\right)\pi+e_n\right)^2\frac{1}{l^2}=\omega_n\sqrt{\frac{\rho A}{EI}} \tag{9}$$

Or $$\omega_n=\left(\left(\frac{2n-1}{2}\right)\pi+e_n\right)^2\frac{1}{l^2}\sqrt{\frac{EI}{\rho A}} \tag{10}$$

2.1. Mass-resonant frequency shift relation for fixed free SWBNNT based biosensor

The variation of added/attached mass in terms of different types of bacterium or viruses to sensor system causes shift to the resonant frequency. The key issue of mass based detection of considered bacterium/viruses is in quantifying the shift in resonant frequency due to additional mass of bacterium/viruses on nanotube. The resonant frequency shift is given by,

$$\Delta f = f_0 - f \tag{11}$$

Where f0 is resonant frequency with no attached mass and f is resonant frequency with attached mass.The minimum sensitivity $S_{\mathrm{minfixedfreebeam}}$for fixed free beam can be given as [Panchal et al. (2013)],

$$S_{\mathrm{min\,fixedfreebeam}} = \frac{\rho A L 4\pi}{15.139\phi} \tag{12}$$

Here,

$$\phi = \sqrt{\frac{EI}{\rho A}}$$

Where E is Young’s modulus of elasticity, I is moment of inertia, A is area and ρ is density of fixed free beam.

3. Continuum solid modeling of SWBNNT

The overall resonant behaviour of SWBNNT based biosensor system has been analyzed considering the equivalent continuum solid modeling based FEM simulation approach [Sohlberg et al. (1998) and Liu et al. (2003)]. Present analysis combines the continuum mechanics in conjunction with FEM simulation package ANSYS to perform the vibration analysis of SWBNNT based biosensor system. The resonant frequency based analysis has been performed considering modal analysis of simulated fixed free SWBNNT based biosensor systems. Among nanotubes, the combination of strong linear bending force acting along longitudinal axis of the nanotube results in inequality between magnitudes of inter atomic forces and ultimately ends up in anisotropic relation [Panchal et al. (2012a, 2012b)]. An assumption is made for SWBNNT which states that linear forces acting along length of nanotubes and thereby considered as transversely isotropic material which is isotropic about one axis [Akin(2005)].This assumption leads to the compliance matrix of 9 terms of which 5 are independent.

For simplicity, the cylindrical coordinate system is employed to simulate the SWBNNT based biosensor system for FEM based modal analysis. The constitutive relation can be obtained as [Panchal et al. (2012a, 2012b)],

$$\begin{Bmatrix} \sigma_r \\ \sigma_\theta \\ \sigma_z \\ \tau_{\theta z} \\ \tau_{rz} \\ \tau_{r\theta} \end{Bmatrix} = \begin{bmatrix} D_{11} & D_{12} & D_{13} & 0 & 0 & 0 \\ D_{12} & D_{22} & D_{23} & 0 & 0 & 0 \\ D_{13} & D_{23} & D_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & D_{22}-D_{33} & 0 & 0 \\ 0 & 0 & 0 & 0 & D_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & D_{66} \end{bmatrix} \begin{Bmatrix} \varepsilon_r \\ \varepsilon_\theta \\ \varepsilon_z \\ \gamma_{\theta z} \\ \gamma_{rz} \\ \gamma_{r\theta} \end{Bmatrix} \tag{13}$$

Where Dij corresponds to stiffness coefficients. The material properties of SWBNNT are considered as; the elastic modulus of 1.22 ± 0.24 TPa [Chopra et al. (1998)], transverse modulus of 30 GPa and Poisson’s ratio of 0.35, to estimate the stiffness coefficients. The mass density ρ has been considered as 2180 kg/m3 [Chopra et al. (1998),Panchal et al. (2012a) and Panchal et al. (2013)]. The stiffness coefficients are take as per Appendix A as an input data for the continuum solid modeling based simulation approach [Panchal et al. (2012a, 2012b)].

The nanoscale attached mass at the tip of fixed free nanotube, in terms of bacterium or viruses is simulated by increasing the length of the nanotube at free end (as shown in fig. 2). The attached mass has been taken as an additional length of same diameter and thickness of SWBNNT.

The increase in length L1, has been calculated as,

$$L_1 = \frac{m_{massattached}}{\rho A} \tag{14}$$

Where $m_{massattached}$ is mass attached at free end of fixed free beam.

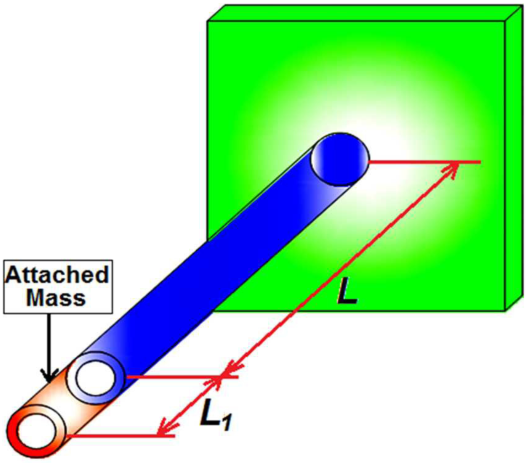

Fig. 2. Fixed free SWBNNT based sensor system with attached mass of length L1.

4. Results and discussion

The aim of present study is to validate the feasibility of SWBNNT based biosensor system in order to identify the bacterium or viruses that are attached to the free end of fixed free SWBNNT. For the present resonant frequency based analysis of SWBNNT based biosensor system, information regarding the masses of various bacterium or viruses to be attached are need to be known. These are available in monographs of Frankel-Conrat (1985), Gunsalus and Stainer (1960) and Elishakoff et al. (2011). The various considered bacterium or viruses used in present study are mentioned in Table 1.

Table 1. Various bacterium or viruses used in study

Type	Bacterium/Viruses	Mass (in kg)
v1	Orthomyxoviridae	6.23E-22
v2	Togoviridae (Smallest)	2.25E-22
v3	Polyoma	6.30E-23
v4	Staphilococcus	5.60E-23
v5	Togoviridae (Largest)	4.19E-23
v6	Caliciviridae	3.94E-23
v7	Nudaurelia	2.90E-23

Table 2. Properties of SWBNNT of considered length having wall thickness of 0.065 nm.

Diameter	Length	Mass(kg)	Fundamental frequency(MHz)	Minimum sensitivity(kg/Hz) (As per Equation 12)
2 nm	2.0 µm	1.72E-21	2.264	8.84E-17
2 nm	1.5 µm	1.29E-21	4.025	6.63E-17
2 nm	1.0 µm	8.62E-22	9.057	4.42E-17
2 nm	0.5 µm	4.31E-22	36.228	2.21E-17

The nanotubes of different length 2.0 μm, 1.5 μm, 1.0 μm and 0.5 μm are considered with each nanotube possessing diameter of 2 nm and effective wall thickness of 0.065 nm. Table 2 summarizes the properties of considered different nanotubes.

Figure 3 shows, the analytical results of first three modes of vibrations for considered different lengths of nanotubes. The analytical results are obtained considering each nano tube as isotropic material with density of 2180 kg/m3 and Young's modulus 1.22 TPa. The obtained results indicate that as length of the nanotube increases the excitation resonant frequency decreases for all three modes of vibration.

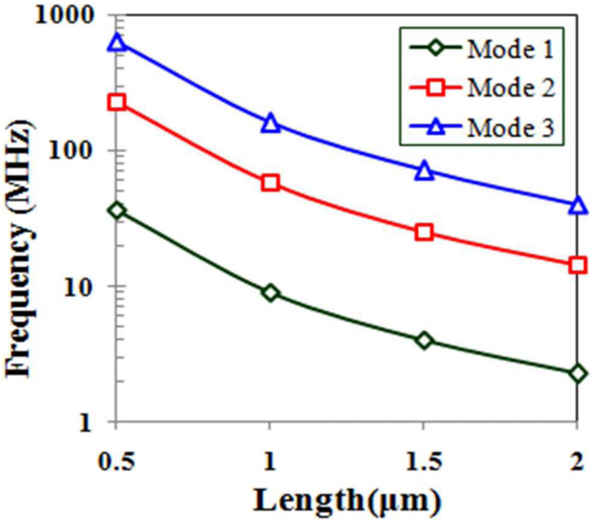

Fig. 3. First three modes of resonant frequency for various considered nanotubes.

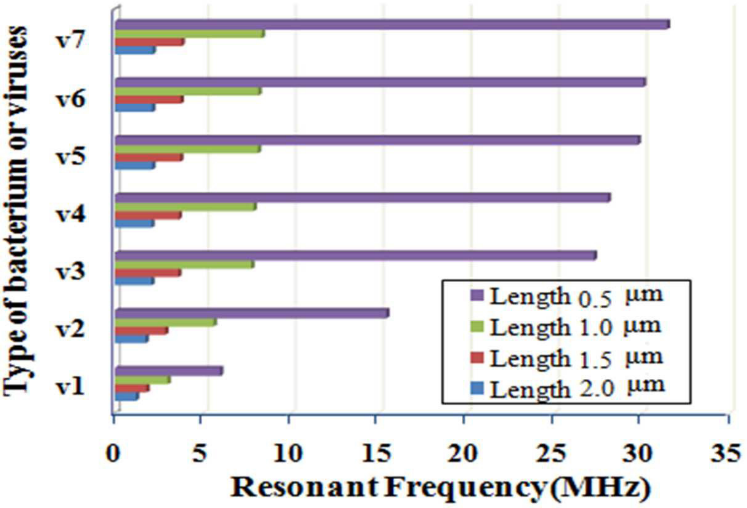

Fig. 4. Variation in resonant frequency due to attached bacterium or viruses at free end of fixed free SWBNNT based biosensor system of different considered lengths.

The resonant frequency variation based analysis is performed for different considered lengths. Figure 4 shows, the obtained continuum solid modeling based simulation results of resonant frequency variation due to attached various bacterium or viruses at free end of fixed free SWBNNT. The difference in simulated results and analytical results of resonant frequency variation because of various bacterium or viruses attached at free end of fixed free SWBNNT is summarized in Table 3, which indicates the percentage error in simulated results and analytical results. It is clear from Table 3 that continuum solid modeling based simulation results are in sensible agreement with analytical results. The variation in percentage error in simulation results is in range of 0.841 to 0.870 with close proximity with the analytical results for the considered lengths of 2.0 µm, 1.5 µm and 1.0 µm. For nanotubes of length 0.5 µm the percentage error vary in the range of 0.860 to 1.027. Which validates the presented continuum solid modeling based simulation approach and can be used for the design of nanomechanical biosensor systems based on SWBNNT.

Table 3. Percentage error in FEM simulated results compared with analytical results.

Type of bacterium or viruses	Mass attached (in kg)	Percentage error in FEM simulated results			
		Length 2.0 µm	Length 1.5 µm	Length 1.0 µm	Length 0.5 µm
Orthomyxoviridae(v1)	6.23E-22	0.841	0.843	0.848	0.860
Togoviridae (Smallest)(v2)	2.25E-22	0.843	0.847	0.858	0.898
Polyoma(v3)	6.30E-23	0.845	0.851	0.869	0.947
Staphilococcus(v4)	5.60E-23	0.844	0.849	0.869	0.950
Togoviridae (Largest)(v5)	4.19E-23	0.845	0.850	0.869	0.958
Caliciviridae(v6)	3.94E-23	0.844	0.851	0.870	0.959
Nudaurelia(v7)	2.90 E-23	0.844	0.850	0.870	1.027

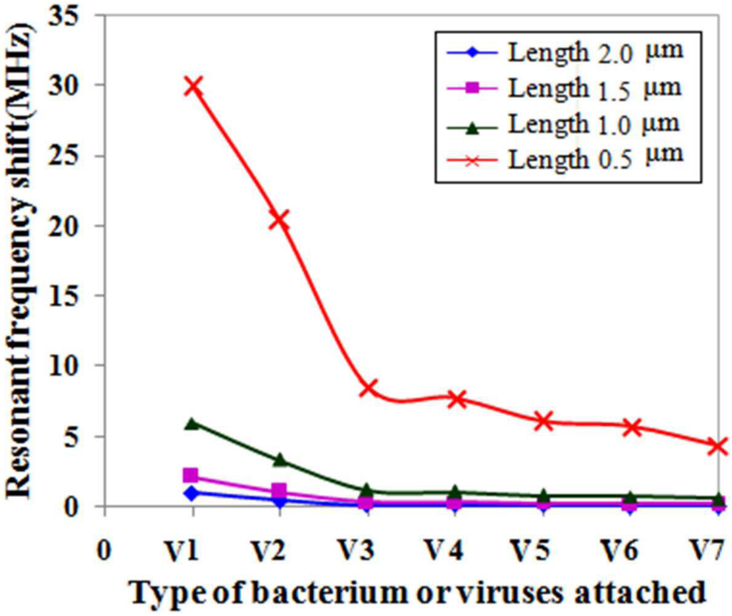

Fig. 5. Variation in frequency shift Δf for various attached considered bacterium or viruses at free end of SWBNNT of different considered lengths.

Figure 5 shows, the variation of frequency shift Δf based on continuum solid modeling based simulation approach for the attached bacterium or viruses at the tip of the fixed free SWBNNT based biosensor system of different considered lengths. It is been observed that frequency shift increases with increase in attached mass in form of bacterium or viruses and also increases as length of nanotube decreases. From the obtained results, it is depicted that resonant frequency shift become larger when nanotubes is shorter. From fig. 5, it is clear that for considered lightest bacterium/virus Nudaurelia (v7) the frequency shift is detectable. As length of nanotubes decreases frequency shift Δ *f* for the lightest bacterium or virus (Nudaurelia) increases. Such variation in resonant frequency shift Δ *f* against variation in size of nanotube suggests that sensitivity of fixed free SWBNNT based biosensor can be improved by scaling down their size.

5. Conclusion

The present work assures the feasibility of SWBNNT based biosensor systems for the possible mass based detection of the considered different bacterium or viruses. The mass based detection of the considered different bacterium or viruses has been performed considering resonant frequency based analysis. The continuum solid modeling based simulation approach is found to be in sensible agreement with continuum mechanics based analytical bending vibration modeling of the fixed free SWBNNT. In order to find out possible enhancement in sensitivity of overall sensor system the variation in frequency shift for different considered lengths of nanotubes has been performed. The obtained results suggest that detection of the bacterium/virus having mass of 2.90 x 10-23 kg can be effectively performed and overall sensitivity of the SWBNNT based biosensor system can be enhanced by scaling down its size.

Appendix A.

Stiffness coefficients for SWBNNT

Stiffness (x 10^9 N/m^2)	
D_{11}	1376.3
D_{12}	16.308
D_{13}	487.4
D_{14}	0
D_{15}	0
D_{16}	0
D_{22}	30.285
D_{23}	16.308
D_{24}	0
D_{25}	0
D_{26}	0
D_{33}	1376.3
D_{34}	0
D_{35}	0
D_{36}	0

D_{44}	14.9
D_{45}	0
D_{46}	0
D_{55}	444.4
D_{56}	0
D_{66}	14.9

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