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STUDY OF HORN SHAPE DOUBLE SINGLE WALLED CARBON NANOTUBE SYSTEM VIA MODIFIED COUPLE STRESS THEORY

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Abstract. In the modern biomedical era of developing nanodevices particularly for the disease detection, fast and precise response is appreciated. Horn shaped double single walled carbon nanotube system (DSWNTS) possess excellent sensing characteristics due to better adsorbing effect. The work here focuses on determination of natural frequency of cantilever type horn shape DSWNTS. As it is already proven fact that such a type is less fragile and more sensitive, noticing its mechanical behavior is the need of time. Here, governing equation of motion pertaining to the dynamic analysis is developed by applying modified couple stress theory using variational principle. The natural frequency is determined and compared with the same of classical theory. The size effect is also discussed. The frequency ratio is more in case of modified couple stress theory particularly with less size effect. This work will be useful in design of low dimension structure for vibration isolation or for mechanical biosensor.
Keywords: DSWNTS; CNT; variational principle; MCST; horn shape.

1. Introduction

Long back, it was beyond mankind’s imagination to sense/grab/identify the molecules floating in the air or to think about a material, which is stronger than regular steel. It was not in reach to have a material which can withstand high pressure and temperature without deformation. All this or even more could be made possible by invention of, a tube of sp^2 hybridized hexagonally arranged carbon atoms, carbon nanotubes (CNTs) in 1991 by a Japanese physicist Sumio Iijima [1]. CNTs have been famed due to their superior capabilities in every field since then [2].

The beauty of nano scale structures lies in their small size irrespective of the shape; be it a wire, rod or a tube. The nanotube may be of different types, namely single walled, double walled, multi walled and may be of different shapes like bamboo, cone, Y and horn shaped. A standard nanotube is uniform in cross-section across entire length whereas horn shaped nanotubes have uniform variation in cross-section across length. They are similar to a frustum of cone in shape i.e. larger diameter at one end and smaller at the other. Among all these shapes of carbon nanotubes, the horn shaped carbon nanotubes (CNTs) have been proved as better sensor as they possess better adsorbing effect. One of the ways for synthesis of cylindrically pointed or horn shaped carbon nanotube [3] uses the chemical vapour deposition cold walled reactor. In this, multi walled CNTs are made by heating up Ni-Co particles so that they deposit on carbon paper at high temperature. Tailoring the morphology of a nanotube opens various frontiers for the wide spread applications like probes for scanning probe microscopy and field emitters, better use in vibration isolation, chemical sensing, nano bio-sensing, electronic nano-devices, nano-opto-mechanical system applications and

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nanocomposites [4]. Authors reported an easier method of making horn shape multi-walled CNTs using carbon tetrachloride as a carbon source and metallic copper as reductant [5]. An idea of making nitrogen doped horn shape CNT was then conceptualized by the reduced reaction of pentachloropyridine with sodium [6]. The temperature in this process reached to 350 °C. If the tapered CNT is grown through thermal catalytic reactions using activated carbon powders in a high temperature resistance furnace, it leads to better yield, stability and alignment [7]. Likewise, there are multiple ways reported for making different shapes of CNTs.

Since the horn shape CNTs are less fragile and more sensitive [8], study of mechanical behavior is essential. Most of the studies in this field consider CNT as a beam element. Various methods (analytical/approximate/experimental/exact) have been utilized for the frequency analysis of tapered beam for different end support conditions like simply supported, clamped [9 – 14]. Only one manuscript is found by authors for study of tapered beam of circular cross-section [13]. This lead to the suitability of thought of having a CNT of tapered cross-section, i.e. horn shape CNT to be used in the bio-sensing application. The analysis of CNT having shape other than regular, has been made with a view of potential applications related to the fracture toughness measurement [15], energy harvesting [16], neural recording [17] and mass sensing [18]. The tapered CNT has opened various frontiers; this study uses the purpose of sensor application with better response time.

A promising direction to develop CNT as a biosensor is to use intermediate materials such as polymers between CNTs. One such simplest nanotube system is DSWNTS, which has two single walled CNTs, attached together with the help of elastic medium [19]. Such a nanotube system may be very well used for acoustic and vibration isolation like macro double beam system [20, 21]. Many nano-scale structures are studied using MCST and the same are given in literature [22 – 27]. Eminent researchers have suggested to use the variational principle approach in accordance with higher order theory to model the governing equations of motion, for nano- and micro-structures, be it static or dynamic [28, 29].

To the best of authors' knowledge, no one has ever reported a combination of horn shape single walled CNTs to make a nanostructure. Combined benefits can be achieved if such a model made using MCST. Present study assumes CNTs equivalent to continuous Euler Bernoulli beams, attached together with a continuous elastic medium. Horn shape DSWNTS has CNTs of horn shape, in which diameter of tube continuously decreases from one end to the other. Such tapered shape provides better sensing capability. A governing equation of motion is developed for the dynamics of horn shape DSWNTS. It is done using modified couple stress theory with variational principle approach. The variation is clearly shown and results are compared with those obtained using classical theory. This work is highly useful to design a low dimension structure for vibration isolation or a mechanical biosensor.

2. Mathematical formulation

This section covers the detailed description of definition of problem. Also, the fundamental of MCST is presented, which is used to model the governing equation to obtain the natural frequency of the horn shape DSWNTS.

Structure of the problem. A combination of two horn shaped single walled carbon nanotubes, attached together with the help of elastic medium (polymer like polyethylene or epoxy), is studied for free vibration analysis in this paper. Both the nanotubes are assumed equivalent to Euler Bernoulli beams of tapered shape. Horn shape DSWNTS has two tapered or horn shaped nanotubes of same bending rigidity (EI), mass (m), length (L) and density (ρ). The stiffness of elastic medium is taken as K. The transverse displacements of two nanotubes are represented by w_1 and w_2, respectively. The Cartesian coordinate system (x, y, z) is adopted for the modeling as represented in Fig. 1 where displacement components *u*, *v* and *w* of displacement vector u; have general representations as that of Euler Bernoulli beam model.

Non-classical theory. It has been a challenging task to shortlist the efficient and appropriate way to solve the problem at nanoscale. The experimental facility is pretty expensive and handling the specimen is a tedious task. On the other hand, the molecular dynamic simulation packages are costly and involve a lot of time due to large amount of data. It is so because each point mass of carbon nanotube is modelled and forces between the bonds are also considered [22]. All this have become limitations of atomistic modelling which can be overcome by using continuum modelling. The classical continuum theories do not consider the parameter of size effect in it. The non-classical theories have emerged as the most effective to handle problems of nanoscale structures due to consideration of size effect. There exists different kind of higher order or non- classical theories. Couple stress theories have come up with the idea of couple stress tensor so as to include the effect of curvature of CNT [23]. Of all, modified couple stress theory (MCST) has only one material length scale parameter to define the small scale effect [24]. Therefore, it is mathematically more convenient and better due to inclusion of symmetric couple stress tensor.

A simplest model to find the transverse deflection, for a single beam of uniform cross-section was presented using MCST [25]. It gave the idea of comparing the result obtained with those of MCST so that importance of this higher order theory could be understood. Likewise, several works have been reported on CNT using modified couple stress theory, only some of them are cited here [26, 27]. Since the commencement of famous MCST by Yang et al. in 2002 [24], the studies of nanostructures are better attempted, than using classical elasticity theory. Symmetric couple stress tensor and one length scale parameter are two most favorable characteristics of this non-classical/higher order theory. According to authors' definition, the strain energy density of a three dimensional isotropic body, occupying the volume Ω is given by [25]

$$U = \frac{1}{2}\int_{\Omega}\left(\sigma_{ij}\varepsilon_{ij} + m_{ij}\gamma_{ij}\right)d\Omega \quad . \tag{1}$$

This strain energy, explained by equation (1), contains the obvious meaningful terms [25] on MCST.

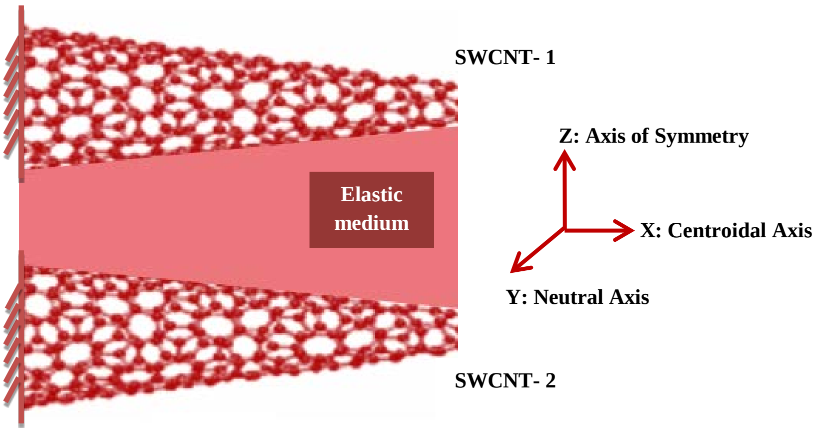


Fig. 1. Horn shaped double single walled carbon nanotube system.

Governing equation of motion. The literature suggests the use of Hamilton's principle to derive the governing equation of motion for any dynamic analysis. Considering horn-shape DSWNTS as a conservative system, Hamilton's principle states that ″the actual solution of any system, among all the paths between two states within a prescribed time interval, keeps the Lagrangian to a minimum value″.

If A_x is the area of cross-section, I_x is the moment of inertia of the cross-section area, the radius function r_x is also a gradient and assumed to be varied as [18]:

$$r_x = \frac{r_0 - r_L}{L} + r_0 = \varepsilon\chi + r_0 \tag{2}$$

$$A_x = \gamma x + n, \qquad \left(\gamma = 2\varepsilon\delta\pi, n = 2\pi r_0 \delta\right) \tag{3}$$

$$I_x = \frac{\pi}{4}\left[\left(r_x + \frac{\delta}{2}\right)^4 - \left(r_x - \frac{\delta}{2}\right)^4\right]. \tag{4}$$

The variation in kinetic energy of the horn shape DSWNTS is given as

$$\delta T = \frac{1}{2}\int_{x=0}^{L} \rho A_x\, \delta\left(\frac{\partial u_1}{\partial t}\right)^2 dx + \frac{1}{2}\int_{x=0}^{L} \rho A_x\, \delta\left(\frac{\partial u_2}{\partial t}\right)^2 dx\ . \tag{5}$$

Strain energy density defined by MCST is given as [25]

$$U = -\frac{1}{2}\int_{x=0}^{L} M_{c_1} \frac{d^2 u_1}{dx^2} dx - \frac{1}{2}\int_{x=0}^{L} M_{c_2} \frac{d^2 u_2}{dx^2} dx + \frac{1}{2} K (u_1 - u_2)^2 \ , \tag{6}$$

where

$$\begin{aligned} M_{c_1} &= M_{x_1} + Y_{xy_1} = -(EI_x + \mu A_x l^2)\frac{d^2 u_1}{dx^2} \\ M_{c_2} &= M_{x_2} + Y_{xy_2} = -(EI_x + \mu A_x l^2)\frac{d^2 u_2}{dx^2} \end{aligned} \tag{7}$$

The variation in work done in the absence of body force is:

$$\delta W = \int_{x=0}^{L} q(x) u_1(x) dx + \int_{x=0}^{L} q(x) u_2(x) dx\ . \tag{8}$$

Application of the Hamilton's principle gives a set of two uncoupled linear differential equations. Let us substitute the following relation for making two uncoupled differential equations coupled [20]:

$$u(x,t) = u_1(x,t) - u_2(x,t)\ . \tag{9}$$

The governing equation of motion is obtained as

$$\frac{d^2}{dx^2}\left(EI_x + \mu A_x l^2\right)\frac{d^2 u}{dx^2} + \rho A_x \frac{d^2 u}{dt^2} + 2Ku = 0\ . \tag{10}$$

The boundary conditions are:

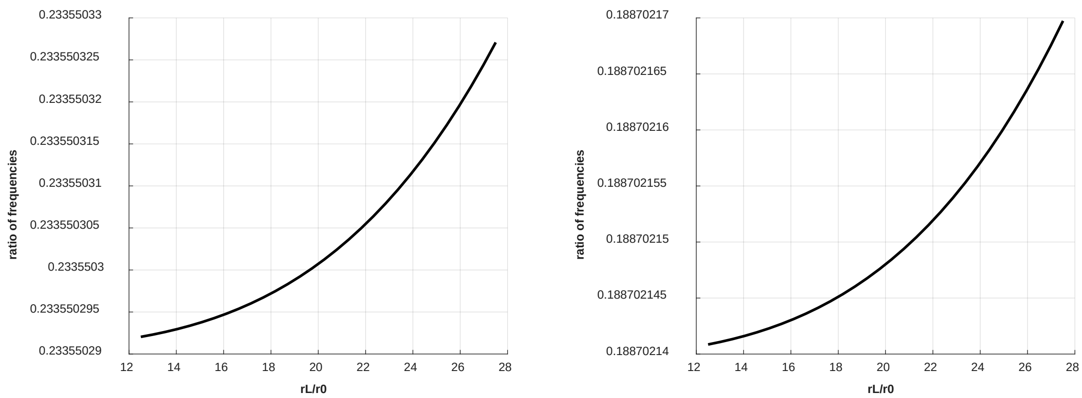
$$u\big|_{x=0} = 0 \qquad u'\big|_{x=0} = 0 \qquad u''\big|_{x=L} = 0 \qquad \left(EI + \mu A l^2\right).u'''\big|_{x=L} = 0\ . \tag{11}$$

Equation (10) is then solved using method of separation of variables and results for natural frequency are plotted for this analytical solution.

3. Result and discussion

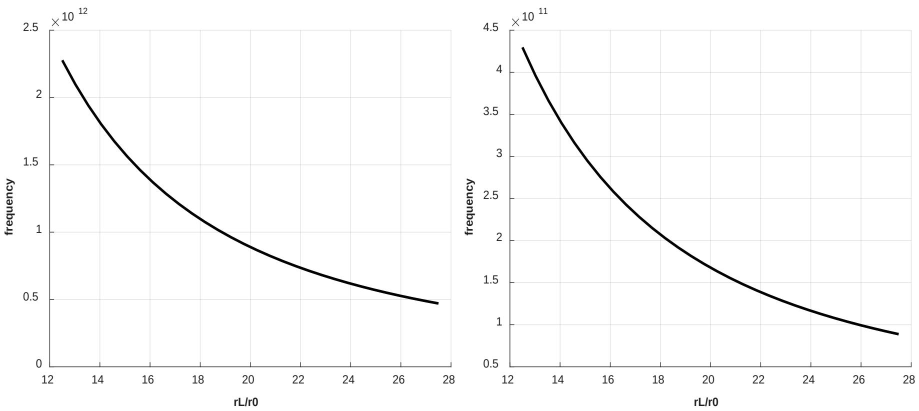
In this section, numerical results are presented for the natural frequency of a horn shape DSWNTS, according to the solution procedure given in Section 2.3. The effect of variation in small length scale parameter and importance of using MCST for a nanostructure are studied. The geometry of the nanostructure under consideration is considered as follow. In the computation, some parameters are used, which are stated here [18]. The Young's modulus (E) is taken as 1 TPa, the mass density (ρ) as 2:24 gm/cm^3, the effective tube thickness (δ) as 0.34 nm, the length of the horn shape SWCNTs (L) as 22 nm, and the radius of the clamped end is taken as 0.8 nm. The radius ratio is taken as $r_L = r_0$, which is assumed to vary from 0.5 to 1. The small length scale parameter (l) in Fig. 3a is taken as 5 nm. All the results shown are for equivalent stiffness K = 5. The poison's ratio υ is assumed as 0.38 [25]. Both the nanotubes are assumed to have the same geometrical and material properties.

The study presented here is for free vibration analysis of horn shape DSWNTS. Fig. 2 depicts the frequency ratios plotted against radius ratio of a horn shape DSWNTS for different size effect. It is found by comparing Fig. 2a and Fig. 2b that the natural frequency of the system becomes higher for the lesser values of material length scale parameter. As it is known, better sensors are better resonators and better resonators are more sensitive to the frequency change even of small amount. Higher frequencies, even for smaller changes on the resonator, make the resonator used as biosensor better. It shows that the system under study is the most efficient resonator, so use as a base for designing a bio-sensing device smaller material length scale parameter (*l*) is always a good decision. It is so due to the length scale parameters in any higher order theory are the responsible agents for considering each point mass in the nanostructure. So, as this value is smaller, more efficient result is found out.



(a) (b)

Fig. 2. Frequency ratio plotted against radius ratio of a horn shape DSWNTS for different size effect: (a) l = 3 nm, (b) l = 5 nm.



(a) (b)

Fig. 3. Natural frequency *vs* radius ratio in case of: (a) MCST, (b) Classical theory.

It is deduced from Fig. 3a and 3b, MCST is a better one to study a nanosystem because it can obtain higher frequency compared to classical theory. Since classical continuum theory does not have a provision of considering atomic distances of nano-scale object, it certainly gives lesser frequency. For the modern biomedical applications, the most sensitive devices are required. So, the structure of such devices must be designed using a higher order theory. This result justifies the applicability of MCST as the involved computation time is less as compared to other higher order theories due to one parameter to consider the size effect. Further, it can be tested for other lengths of SWCNTs and other properties of elastic medium.

Effect of stiffness should also be judged before finally designing the biosensor using this model.

4. Conclusions

In the present study, a model for developing a governing equation of transverse vibration for cantilever type horn shape DSWNTS is developed. This is performed by using MCST variational principle approach. The results show that, the ratio of frequency is greater at lesser value of size effect. Also, the use of non-classical theory gives larger resonance frequency as compared to classical theory. This model is useful to design a biosensor, operated anywhere for judging the presence of any biomolecule.

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