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# Investigation on mechanical vibration of double-walled carbon nanotubes with inter-tube Van der waals forces

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**Abstract.** This work represents the study of the vibration response of the double walled carbon nanotubes (DWCNT) for various boundary conditions. The inner and outer carbon nanotubes are modeled as two individual Euler-Bernoulli's elastic beams interacting each other by Van der waals force. Differential transform method (DTM) is used as a numerical method to solve the governing differential equations and associated boundary conditions. The influence of Winkler elastic medium on vibration frequency is also examined and results are interpreted. MATLAB is used as a tool for solving the governing differential equations. The fundamental natural frequencies are validating with those available in literature and observed a good agreement between them.

**Keywords:** vibration; DWCNT; DTM; winkler; natural frequency

## 1. Introduction

Advanced materials and nano-scale structures with enhanced mechanical, thermal, and electrical properties, such as graphene sheets, are widely used in many nanoelectro-mechanical systems. Thus understanding the dynamic response of these nanostructures is much needed for design and development of a new class of nano-systems such as nano- actuators and nano-sensors.

Iijima's (1991) discovery paper on multi-walled carbon nanotubes led to a major revolution in the area of nano science and nanotechnology. Carbon nanotubes have subjected to much attention as a result of their extending applications in the different emerging fields of nanotechnology.

In aerospace industries, there is a great demand for new materials which show improved mechanical properties i.e., high strength to weight ratio, high thermal stability, and high corrosion resistance. Carbon nanotubes are allotropes of carbon with a cylindrical nanostructure. Nanotubes have been fabricated with l/d ratio of up to 132,000,000:1, significantly larger than any other material (Ball 2001, Rafiee and Moghadam 2014). The structure of a single walled carbon nanotube can be characterized by packaging a one-atom-thick layer of graphite called graphene into a flawless cylinder (Ball 2001, Baughman *et al*. 2002, Qian *et al*. 2002). Carbon nanotubes are capable of withstanding a temperature of 2800°C, which is much higher than the current carbon fiber of 1600°C (Pop *et al*. 2007, Pop *et al*. 2005, Roth and Carroll 2015). Carbon nanotubes are the strongest and stiffest materials yet discovered in terms of the tensile strength and Elastic Modulus respectively (Treacy *et al*. 1996, Stallard *et al*. 2018).

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As carbon nanotubes have very high tensile strength and elastic property. Therefore the vibration and buckling analysis of carbon nanotubes is much essential to get insight in to its capability for industrial applications. By experimental observations, it has been observed that the small-scale effects play a significant role in the physical behavior of nano- structures (Affoune *et al*. 2001, Karličić *et al*. 2015). However, performing experiments on the nano-scale level is not an easy task due to weak control of parameters in the system and high-cost of such research (Frank *et al*. 2007, Thamaraikannan and Pradhan 2016). For this reason, the researchers are focused on developing the theoretical methods. In the branch of theoretical models, two main techniques exist: (i) atomistic models; and (ii) continuum models. Atomistic methods such as deterministic and stochastic molecular dynamics, density function theory etc., are very important and useful for nano-structures composed of a small number of particles (Frank *et al*. 2007). However, for the systems that are composed of a large number of particles, this method is computationally prohibitive (Pei *et al*. 2010, Ansari *et al*. 2010). Due to mentioned demerits of the experimental and atomistic techniques, theoretical models based on continuum theories attracted a great attention of researchers in recent years.

For vibration analysis of one dimensional beam-like structures, Euler–Bernoulli beam model and Timoshenko beam model were usually employed, which assumed that the cross-section of beams remained plane under bending deformation (Wang and Varadan 2006, Murmu and Pradhan 2009a, Ravi Kumar 2017a, Mandal and Pradhan 2014, Jiang *et al*. 2017). Size-dependent continuum-based methods (Murmu and Pradhan 2009b, Bikramsingh and Sankara Subramanian 2017, Kumar and Reddy 2017, Kumar and Deol 2016, Fang *et al*. 2013, Akgöz and Civalek 2016) are becoming popular in modeling small sized structures as it offers much faster and accurate solutions. Hosseini *et al*. (2014) analyzed the vibration of a single-layered graphene sheet introducing the Mindlin plate theory and nonlocal elasticity. Solutions for natural frequencies were obtained in closed form for simply-supported graphene sheets. Recently, some researchers have analyzed nanoplates by utilizing the nonlocal high order shear deformation plate theories (Bounouara *et al*. 2016, Mandal and Pradhan 2014). Yoon *et al*. (2002) analyzed the vibration behaviour of Multi-walled carbon nanotubes utilizing Multiple-elastic beam model and Euler beam theory. They identified the non co-axial vibration response of carbon nanotubes under simply supported boundary condition. Which is determined to agree well with more recent atomistic simulations on the noncoaxial vibration of multi-walled carbon nanotubes (Zhao *et al*. 2003, Li and Chou 2004, Yoon *et al*.2002).

Bikramsingh and Sankara Subramanian (2017), Kumar and Reddy (2017), Ravi Kumar *et al*. (2017), Karličić *et al*. (2015), Tounsi *et al*. (2013) carried out vibration and buckling analysis of single and double -walled carbon nanotubes embedded in an elastic medium and visco-elastic medium. They presented a detailed structural analysis of nanoscale materials and devices. Relevant vibration analyses are reported by many authors in literature by considering both linear and non-linear cases (Gul and Aydogdu 2018, Fernandes *et al*. 2017, Manevitch *et al*. 2017, Askari and Esmailzadeh 2017).

In the present work, differential transform method is used to study the vibration of carbon nanotubes embedded in an elastic medium. Zhou proposed differential transformation method to solve both linear and non-linear initial value problems in electric circuit analysis. Chen and Ho (1999) applied this method to eigen value problems.

Table 1 Differential transformations for mathematical equations

| Original function | Transformed function |
|---|---|
| $y(x) = u(x) \pm v(x)$ | $Y(i) = U(i) \pm V(i)$ |
| $y(x) = \lambda u(x)$ | $Y(i) = \lambda U(i)$ |
| $y(x) = \dfrac{d^n u(x)}{dx^n}$ | $Y(i) = (i+1)(i+2)...(i+n)U(i+n)$ |

## 2. Differential transform method

The differential transform method is a semi-analytical method which is based on the Taylor series expansion. The differential transformation of the $i^{th}$ derivative of the function $u(x)$ is defined as follows

$$U(\mathrm{i}) = \frac{1}{\mathrm{i}!}\left[\frac{d^i u(x)}{dx^i}\right]_{x=x_0} \quad (1)$$

And the differential inverse transformation of $U(i)$ is expressed as

$$u(x) = \sum_{i=0}^{\infty} U(\mathrm{i})(x - x_0)^i \quad (2)$$

In real application function, $u(x)$ is expressed as finite series and Eq. (2) can be written as

$$u(x) = \sum_{i=0}^{n} U(\mathrm{i})(x - x_0)^i \quad (3)$$

Now using certain transformation rules we can convert the governing differential equation and associated Boundary Conditions into some algebraic equations and after solving them we can get the desired results. We can use the following transformation table for this purpose.

## 3. Formulation

Based on the Euler–Bernoulli beam model, the governing equation of motion of a beam is given by

$$\rho A \frac{\partial^2 w}{\partial t^2} + EI \frac{\partial^4 w}{\partial^4 x} = P(\mathrm{x}) \quad (4)$$

Where $x$ and $t$ are the axial coordinate and time, respectively. $w(x, t)$ and $p$ are the deflection of carbon nanotubes and the distributed transverse force acted on the nanotubes, respectively. $E$ and $I$ are the elastic modulus and the moment of inertia of a cross-section, respectively. $A$ is the cross-sectional area and $\rho$ is the mass density of nanotubes.

For the double walled carbon nanotubes, the interaction between inner and outer nanotubes is considered to be coupled together through the Van der Waals (vdW) forces. Eq. (4) can be applied to each layer of the inner and outer nanotubes of the double-walled carbon nanotubes. Thickness of inner and outer nanotubes is assumed to be constant. Based on the Euler-Bernoulli beam model, we have

$$\rho A_1 \frac{\partial^2 w_1}{\partial t^2} + EI_1 \frac{\partial^4 w_1}{\partial^4 x} = p_1 \tag{5}$$

$$\rho A_2 \frac{\partial^2 w_2}{\partial t^2} + EI_2 \frac{\partial^4 w_2}{\partial^4 x} = p_2 \tag{6}$$

Where, the subscripts 1 and 2 denote the quantities associated with the inner and outer nanotubes respectively.

The pressure $P_1$ acting on the inner nanotube is due to the van der waals interaction is given by

$$p_1 = c(w_2 - w_1) \tag{7}$$

Where, $c$ is the *vdW* interaction coefficient between inner and outer nanotubes.

The pressure acting on the outer layer due to the surrounding elastic medium can be given by

$$p_w = -kw_2 \tag{8}$$

Where negative sign indicates that $p_w$ is in the direction opposite to the deflection of nanotubes. $k$ is the spring constant.

Thus, for the embedded DWCNTs, the pressure of the outer nanotube supported by the elastic medium is given by

$$p_2 = p_w - c(w_2 - w_1) \tag{9}$$

In the model Van der waals interaction (*vdW*) coefficient ($c$) can be obtained from the interlayer energy potential, given as (He *et al*. 2006)

$$c = \frac{\pi \varepsilon R_1 R_2 \sigma^6}{a^4} \left[ \frac{1001\sigma^6}{3} H^{13} - \frac{1120}{9} H^7 \right] \tag{10}$$

where

$$H^m = (R_1 + R_2)^{-m} \int_0^{\pi/2} \frac{d\theta}{(1 - KCos^2\theta)^{m/2}}, (m = 7,13)$$

And

$$K = \frac{4 R_1 R_2}{(R_1 + R_2)^2}$$

Here $a$ = 0.142 nm (carbon to carbon atom bond length). $R_1$, $R_2$ are the inner and outer radii of double walled carbon naotubes. $\sigma$ = 0.34 nm, $\varepsilon$ = 2.967 meV are the *vdW* radius and the well depth of Lennard-Jones potential respectively as given by Saito *et al*. (2001).

Thus

$$\rho A_1 \frac{\partial^2 w_1}{\partial t^2} + EI_1 \frac{\partial^4 w_1}{\partial^4 x} = c(w_2 - w_1) \tag{11}$$

$$\rho A_2 \frac{\partial^2 w_2}{\partial t^2} + EI_2 \frac{\partial^4 w_2}{\partial^4 x} = -kw_2 - c(w_2 - w_1) \tag{12}$$

In this analysis, we consider that the deflection of double walled carbon nanotubes has different vibrational modes, $W_j(x), j = 1, 2$ for the inner and outer nanotubes.

$$w_j(x,t) = W_j(x)e^{i\omega t} \tag{13}$$

Using the Table 1, the differential transformation of Eqs. (11) and (12) can be written as

$$W_1(i+4) = \frac{(\beta(W_2(i) - W_1(i) + r.W_1(i))}{(i+1)(i+2)(i+3)(i+4)} \tag{14}$$

$$W_2(i+4) = \frac{((\beta/\delta)(W_1(i) - W_2(i)) + r(\eta/\delta).W_1(i) - (\bar{k}/\delta)\,\mathrm{W}_2(\mathrm{i}))}{(i+1)(i+2)(i+3)(i+4)} \tag{15}$$

Where

$$r = \frac{\rho A_1 \omega^2 L^4}{EI_1}, \qquad \beta = \frac{cL^4}{EI_1}, \qquad \eta = \frac{A_2}{A_1}, \qquad \delta = \frac{I_2}{I_1}, \qquad \bar{k} = \frac{kL^4}{EI_1},$$

The above equations can be solved for natural frequency by using the appropriate boundary conditions and transformed boundary conditions.

### *3.1 Boundary conditions*

*SIMPLY SUPPORTED CNTs*

For the simply supported CNT beam boundary conditions at both ends are defined mathematically as

$$w_1 = 0, \quad \frac{d^2 w_1}{dx^2} = 0, \quad w_2 = 0, \quad \frac{d^2 w_2}{dx^2} = 0 \tag{16}$$

*CLAMPED-CLAMPED CNTs*

For clamped-clamped CNT case, the boundary conditions at both ends are defined as

$$w_1 = 0, \quad \frac{dw_1}{dx} = 0, \quad w_2 = 0, \quad \frac{dw_2}{dx} = 0 \tag{17}$$

*CLAMPED-HINGED CNTs*

For clamped-hinged CNT case, the boundary conditions are defined as

At $x = 0$

$$w_1 = 0, \quad \frac{dw_1}{dx} = 0, \quad w_2 = 0, \quad \frac{dw_2}{dx} = 0 \tag{18}$$

At $x = L$

$$w_1 = 0, \quad \frac{d^2 w_1}{dx^2} = 0, \quad w_2 = 0, \quad \frac{d^2 w_2}{dx^2} = 0 \tag{19}$$

## 4. Results and discussions

### 4.1 Comparison with analytical solutions

In this study, we consider double walled carbon nanotubes embedded in a Winkler medium. Nanotubes are having the inner and outer diameters of 4.8 nm and 5.5 nm, respectively. The effective thickness of each nanotube is taken to be as 0.34 nm. The elastic modulus of carbon nanotube is 1 TPa and the density is considered as 2.3 g/cm$^3$ (Elishakoff and Pentaras 2009).

By using the differential transformation method as the numerical method the natural frequency for double walled carbon nanotubes has been computed. Results are compared and interpreted.

From Tables 2-3 it is clearly observed that fundamental frequency of double walled carbon nanotubes is decreasing with increasing aspect ratio ($L/d$, where $d$ = diameter of the outer nanotube) of nanotubes.

Table 2 DWCNTs fundamental frequency in THz for simply supported ends

| *L*/*d* | 10 | 12 | 14 | 16 | 18 | 20 |
|---|---|---|---|---|---|---|
| Present [DTM] | 0.46830 | 0.32527 | 0.23899 | 0.18298 | 0.14467 | 0.11716 |
| Exact (Elishakoff and Pentaras 2009) | 0.46830 | 0.32527 | 0.23899 | 0.18298 | 0.14467 | 0.11716 |
| Bubnov (Elishakoff and Pentaras 2009) | 0.47211 | 0.32791 | 0.24093 | 0.18447 | 0.14576 | 0.11806 |
| Petrov (Elishakoff and Pentaras 2009) | 0.46884 | 0.32564 | 0.23926 | 0.18319 | 0.14475 | 0.11725 |
| (Xu *et al*. 2006) | 0.46 | ……. | ……. | …….. | …….. | 0.11 |

Table 3 Clamped-clamped DWCNTs fundamental frequency in THz

| *L*/*d* | 10 | 12 | 14 | 16 | 18 | 20 |
|---|---|---|---|---|---|---|
| Present [DTM] | 1.06406 | 0.73683 | 0.54256 | 0.41371 | 0.32654 | 0.26546 |
| Bubnov ( Elishakoff and Pentaras 2009) | 1.07986 | 0.75063 | 0.55171 | 0.42248 | 0.33385 | 0.27043 |
| Petrov ( Elishakoff and Pentaras 2009) | 1.06478 | 0.73087 | 0.54341 | 0.41135 | 0.32505 | 0.26331 |
| (Xu *et al*. 2006) | 1.06367 | …… | …… | ……. | ……. | 0.2660 |

### *4.2 Influence of surrounding medium on vibration frequencies of DWCNTs*

Now if we change the value of Winkler Elasticity constant ($k$) from 0-300 GPa and $L$ = 20 nm, we can obtain different values of vibration frequencies which are shown below.

Influence of the surrounding medium on the vibration frequency is investigated based on the Winkler spring model. From Figs. 1-3, it can be found that vibration frequencies of the embedded double walled carbon nanotubes are larger than those of the nested double walled carbon nanotubes. Especially, the influences of surrounding medium on the vibration frequency are significant for the first in-phase modes while on the other hand stiffness of surrounding medium impacts very little on the vibration frequencies of the anti-phase modes.

### *4.3 Vibration amplitude ratio ($Y_1/Y_2$) of inner and outer nanotubes*

Tables 4-6 represent the vibration amplitudes of inner and outer nanotubes for various boundary conditions.

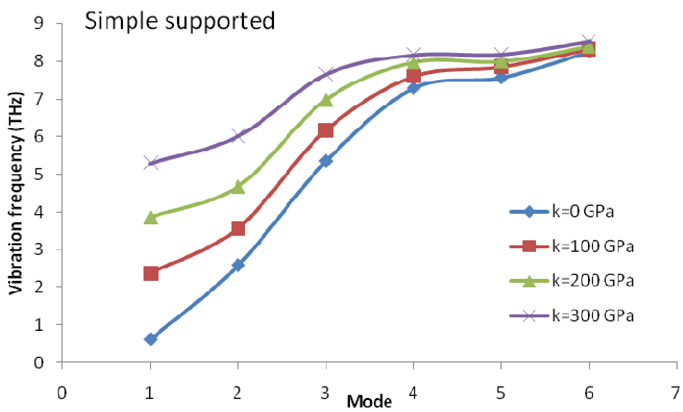


Fig. 1 Influence of winkler foundation on vibration frequencies for simply supported DWCNTs

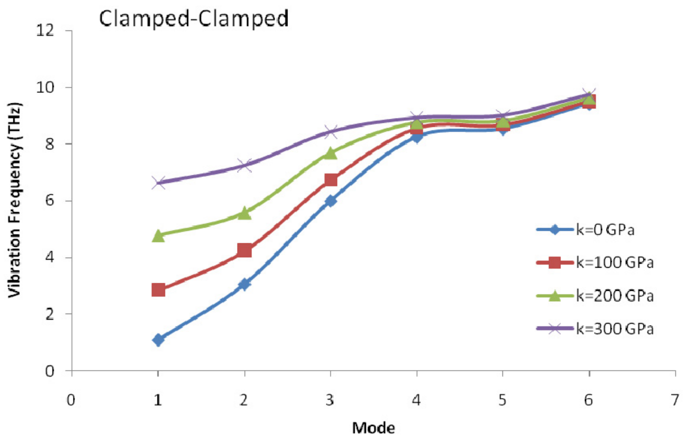


Fig. 2 Influence of winkler foundation on vibration frequencies for clamped-clamped DWCNTs

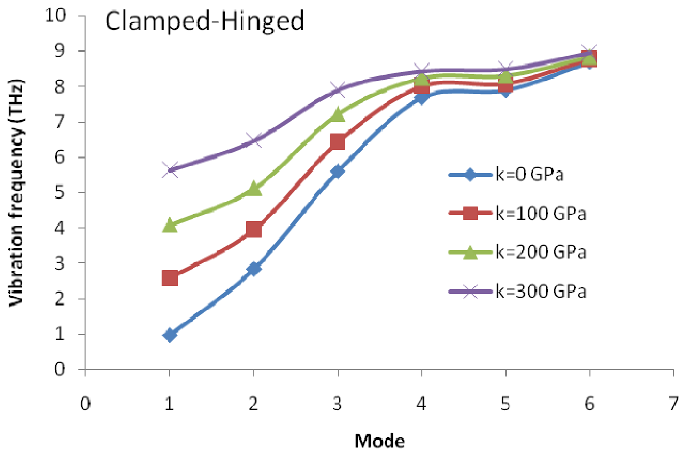


Fig. 3 Influence of winkler foundation on vibration frequencies for clamped-hinged DWCNTs

Table 4 Amplitude ratio of the inner to outer nanotubes for Simple-supported DWCNTs

| Mode | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| Frequency (THz) | 0.618 | 2.586 | 5.447 | 7.283 | 7.564 | 8.248 |
| $Y_1 / Y_2$ | 1.000 | 1.130 | 1.438 | 2.183 | -0.546 | -0.664 |

Table 5 Amplitude ratio of the inner to outer nanotubes for Clamped - Hinged DWCNTs

| Mode | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| Frequency (THz) | 0.968 | 2.84 | 5.601 | 7.684 | 7.892 | 8.695 |
| $Y_1 / Y_2$ | 1.010 | 1.134 | 1.597 | 2.210 | -0.740 | -0.862 |

Table 6 Amplitude ratio of the inner to outer nanotubes for Clamped - Clamped DWCNTs

| Mode | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| Frequency (THz) | 1.08 | 3.046 | 5.988 | 8.245 | 8.526 | 9.424 |
| $Y_1 / Y_2$ | 1.023 | 1.153 | 1.692 | 2.362 | -0.964 | -1.020 |

Out of all these (Tables 4-6) boundary conditions, clamped –clamped boundary condition has the highest natural frequencies. In anti-phase mode there are very little variations in fundamental frequencies. These observations may be useful for the designer to estimate the fundamental natural frequencies in each two series.

## 5. Conclusions

In this study, the vibration analysis of double walled carbon nanotubes embedded in an elastic medium for various boundary conditions is studied by using a numerical technique called differential transform method in a simple and accurate way. Results show that phase modes have a strong dominance on natural frequencies of carbon nanotubes. The stiffness of surrounding medium is also studied which shows that it has significant effect on the vibration frequencies of double walled carbon nanotubes for the first in-phase modes and represents very little effect on frequencies in anti-phase modes.

The investigation presented may be helpful in the application of carbon nanotubes such as high-frequency oscillators, dynamic mechanical analysis and mechanical sensors.

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