

## FREE VIBRATION ANALYSIS OF DOUBLE-WALLED CARBON NANOTUBES EMBEDDED IN AN ELASTIC MEDIUM USING DTM (DIFFERENTIAL TRANSFORMATION METHOD)

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### Abstract

The study of vibration in carbon nanotubes (CNTs) is currently a major topic of interest that increases understanding of their dynamic mechanical behavior. By now, there are three methods to analyze the mechanical properties of carbon nanotube (CNT). They are spectroscopy experiment, computational simulation, and theoretical analysis. However, technically these are difficult experiments of vibrational properties because of the small diameter of the nanotubes, and plenty of time will be spent on the molecular dynamics (MD) simulation. Theoretical analyses have shown the advancement of the taken cost and the spent time of researches compared with the experimental operation and molecular dynamic (MD) simulation method, and they can predict some results which cannot be achieved by the other two methods by now. Elastic continuum models are used to study the vibrational behavior of carbon nanotubes to avoid the difficulties encountered during experimental characterization of nanotubes as well as the time-consuming nature of computational atomistic simulations. To calculate the resonant vibration of double-walled carbon nanotubes (DWCNTs) embedded in an elastic medium, a theoretical analysis is presented based on Euler-Bernoulli beam model and Winkler spring model.

Keywords: Buvnov-Galerkin, Differential transformation method (DTM), Double-walled carbon nanotubes (DWCNTs), MATLAB, Petrov-Galerkin.

### 1. Introduction

Extensive research work has been carrying out on analysis of carbon nanotube due to their high mechanical, electrical and thermal properties [1-4] over other materials. Since it was discovered by Iijima [1], various models have been used

**Nomenclatures**

$A$	Area of carbon nanotube, $m^2$
$c$	Van der Waals interaction coefficient
$E$	Elastic modulus of carbon nanotubes, TPa
$I$	Moment of inertia about the neutral axis, $m^4$
$k$	Elasticity of Winkler's medium, GPa
$L$	Length of carbon nanotube, m
$w$	Transverse deflection of carbon nanotube, m

**Greek Symbols**

$\omega$	Natural frequency of carbon nanotube, THz
$\rho$	Density of carbon nanotube, $kg/m^3$
$\Omega$	Non-dimensional frequency
$\delta$	Ratio of moment of inertia of outer and inner carbon nanotube

**Abbreviations**

C-C	Clamped-Clamped
C-H	Clamped-Hinged
CNT	Carbon Nanotube
DTM	Differential transformation method
DWCNT	Double-Walled Carbon Nanotube
S-S	Simply Supported

to analyse nanostructures theoretically beside experimentally. The atomistic models are the more accurate but the computational cost and time are high for the relatively large-scale nanostructures. Alternatively, the continuum models provide faster and approximate results.

Carbon nanotubes are the allotropes of carbon with a cylindrical nanostructure. Nanotubes have been constructed with a length-to-diameter ratio up to 132,000,000:1, significantly larger than any other material [1, 2]. This is because of very strong  $sp^2$  carbon-carbon bond between the atoms. These cylindrical carbon molecules have novel properties, making them potentially useful in many applications in nanotechnology, electronics, optics, and other fields of materials science, as well as potential uses in aerospace fields [3]. Many believe that CNTs would provide the ultimate reinforcing materials for the development of a new class of nanocomposites [4, 5]. Experiments show that carbon nanotubes have extraordinary electrical [6], thermal [7] and mechanical properties [2, 3, 8]. Mechanically, CNTs have a tensile strength that is twenty times that of high strength steel and Young's modulus in the order of a terra Pascal [8]. Mechanical properties of carbon nanotubes are given in Table 1. Several studies related to bending, buckling, and vibration of single walled and double walled carbon nanotubes have been reported in literature [9-12].

In the present work, differential transformation method has been used to study the vibration of carbon nanotube with nonlocal effect. Zhou [13] proposed differential transformation method to solve both linear and non-linear initial value problems in electric circuit analysis. Later Chen and Ho [14] applied this method to eigen value problems. Aydogdu [15] applied differential transformation method to solve the intergro – differential equation.

The superiority of the DTM is its simplicity and good precision and depends on Taylor series expansion while it takes less time to solve polynomial series. It is different from the traditional high order Taylor's series technique, which needs symbolic computation of the necessary derivatives of the data functions. The Taylor series method takes relatively long time for computations involving large orders. With DTM technique, it is also possible to compute near exact solutions for differential equations.

**Table 1. Comparison of mechanical properties of CNTs [16].**

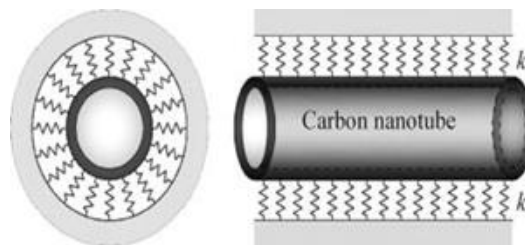
Material	Young's modulus (TPa)	Tensile strength (GPa)	Elongation at break (%)
SWCNT	~1 (from 1 to 5)	13–53	16
Stainless Steel	0.186–0.214	0.38–1.55	15–50
DWCNTs	from 2 to 8	16–65	12

## 2. Formulation

The continuum mechanics method has been successfully applied to analyze the dynamic responses of individual carbon nanotubes. Based on the Euler–Bernoulli beam model, the governing equation of motion of a beam is given by [17].

$$\rho A \frac{\partial^2 w}{\partial t^2} + EI \frac{\partial^4 w}{\partial x^4} = P(x) \quad (1)$$

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



**Fig. 1. Analysis model of CNTs embedded in the elastic medium.**

Figure 1 shows the analysis model carbon nanotubes embedded in an elastic medium. The stiffness of the spring medium is  $k$ .

For the double-walled carbon nanotubes, the interaction between inner and outer nanotubes is considered to be coupled together through the van der Waals forces.

Equation (1) can be used to each layer of the inner and outer nanotubes of the double-walled carbon nanotubes, assuming that the inner and outer nanotubes have the same thickness and effective material constants. Based on the Euler–Bernoulli beam model, we have:

$$\rho A_1 \frac{\partial^2 w_1}{\partial t^2} + EI_1 \frac{\partial^4 w_1}{\partial x^4} = P_1 \quad (2)$$

$$\rho A_2 \frac{\partial^2 w_2}{\partial t^2} + EI_2 \frac{\partial^4 w_2}{\partial x^4} = P_2 \quad (3)$$

where, the subscripts 1 and 2 denote the quantities associated with the inner and outer nanotubes, respectively.  $P_j$  ( $j=1, 2$ ) are the pressures exerted on inner and outer nanotubes.

For small deflection linear vibration, the interaction pressure at any point between the two adjacent nanotubes depends linearly on the difference of their deflections at that point.

Thus, the pressure  $P_1$  acting on the inner nanotube caused by van der Waals interaction is given by

$$P_1 = c(w_2 - w_1) \quad (4)$$

where  $c$  is the van der Waal interaction coefficient between inner and outer nanotubes.

Winkler spring model has been widely used to analyse the mechanical properties of embedded carbon nanotubes. The pressure acting on the outermost layer due to the surrounding elastic medium can be given by

$$P_w = -k w_2 \quad (5)$$

where negative sign indicates that  $P_w$  is in the opposite direction of the deflection of nanotubes.

Thus, for the embedded double-walled carbon nanotubes, the pressure of the outermost nanotube contacting with the elastic medium is given by

$$P_2 = P_w - c(w_2 - w_1) \quad (6)$$

In the simulation van der Waal interaction coefficient ( $c$ ) can be obtained from the interlayer energy potential, given as [18]

$$c = \frac{320(2R_1)}{0.16d^2} \frac{\text{erg}}{\text{cm}^2}, d = 0.142 \text{ nm} \quad (7)$$

where,  $R_1$  = Radius of the inner nanotube.

Thus, by using Eqs. (4), (6) and (7) we have,

$$\rho A_1 \frac{\partial^2 w_1}{\partial t^2} + EI_1 \frac{\partial^4 w_1}{\partial x^4} = c(w_2 - w_1) \quad (8)$$

Similarly, for the second nanotube, the governing equation can be written as:

$$\rho A_2 \frac{\partial^2 w_2}{\partial t^2} + EI_2 \frac{\partial^4 w_2}{\partial x^4} = -k_w - c(w_2 - w_1) \quad (9)$$

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

The displacements of the vibrational solution in double-walled carbon nanotubes can be given by

$$w_j(x, t) = W_j(x).e^{i\omega t} \quad (10)$$

Equations (8) and (9) can be further simplified as:

$$\frac{d^4 \bar{W}_1}{dX^4} - \Omega^2 \bar{W}_1 = \beta(\bar{W}_2 - \bar{W}_1) \quad (11)$$

$$(\delta) \frac{d^4 \bar{W}_2}{dX^4} - \eta \Omega^2 \bar{W}_2 = \beta(\bar{W}_1 - \bar{W}_2) - \bar{k} \bar{W}_2 \quad (12)$$

where

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

### 3. Differential Transform Method (DTM) and Solution Procedure

Differential transformation method is based on Tayler series expansion. In this technique, the governing equation, and the boundary conditions are transformed into a set of algebraic simultaneous equations.

By solving these equations, one can obtain the governing equation's solution with great accuracy [14].

$$y(x) = \sum_{i=0}^n \frac{x^i}{i!} \left[ \frac{d^i y(x)}{dx^i} \right]_{x=0} \quad (13)$$

where the value of  $n$  (the number of iterations) is determined by the convergence requirement in the study.

The simplicity of the solutions of the algebraic equations is remarkable because equations can be solved very quickly using the symbolic computational software, MATLAB.

Equations (11) and (12) can be solved for natural frequency by using the appropriate boundary conditions and transformed boundary conditions. We can use the following transformation (referring to Table 2) for this purpose.

**Table 2. Differential transformations for mathematical equations.**

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

### 3.1. Application of DTM

By using Table 2, the differential transformation of Eqs. (11) and (12) can be written as

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

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

$$\text{where, } r = \frac{\rho A_1 \omega^2 L^4}{EI_1}.$$

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

### 3.2. Simply supported double - walled carbon nanotubes

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

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

By using Table 2, differential transformation of the above boundary conditions can be written as

$$W_1(0) = 0, W_1(2) = 0, W_2(0) = 0, W_2(2) = 0 \quad (17)$$

$$\sum_{i=0}^{\infty} W_1(i) = 0, \sum_{i=0}^{\infty} i(i-1)W_1(i) = 0, \sum_{i=0}^{\infty} W_2(i) = 0, \sum_{i=0}^{\infty} i(i-1)W_2(i) = 0 \quad (18)$$

By assuming  $W_1(1) = c_1$ ,  $W_1(3) = c_2$ ,  $W_2(1) = c_3$ ,  $W_2(3) = c_4$ , one can calculate  $W_1(i)$ ,  $W_2(i)$  up to  $n$  terms from the Eqs. (14) and (15) and it will be substituted in Eqs. (17) and (18) and by solving these four equations for a non-trivial solution, one gets natural frequency ( $\omega$ ) of the CNTs. The accuracy of natural frequency increases with increasing the value of  $n$  (number of iterations) and saturates after certain  $n$  value.

### 3.3. Clamped-clamped double- walled carbon nanotubes

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

$$w_1 = 0, \frac{dw_1}{dx} = 0, w_2 = 0, \frac{dw_2}{dx} = 0 \quad (19)$$

Differential transformation of the above boundary conditions can be written as:

$$W_1(0) = 0, W_1(1) = 0, W_2(0) = 0, W_2(1) = 0 \quad (20)$$

$$\sum_{i=0}^{\infty} W_1(i) = 0, \sum_{i=0}^{\infty} i.W_1(i) = 0, \sum_{i=0}^{\infty} W_2(i) = 0, \sum_{i=0}^{\infty} i.W_2(i) = 0 \quad (21)$$

By assuming  $W_1(2) = c_1$ ,  $W_1(3) = c_2$ ,  $W_2(2) = c_3$ ,  $W_2(3) = c_4$  the Eqs. (14) and (15) can be calculated up to  $n$  terms and a similar procedure is followed as that of simply supported boundary condition.

### 3.4. Clamped-Hinged double-walled carbon nanotubes

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

At  $x=0$

$$w_1 = 0, \frac{dw_1}{dx} = 0, w_2 = 0, \frac{dw_2}{dx} = 0 \quad (22)$$

At  $x=L$

$$w_1 = 0, \frac{d^2w_1}{dx^2} = 0, w_2 = 0, \frac{d^2w_2}{dx^2} = 0 \quad (23)$$

Differential transformation of the above boundary conditions can be written as:

At  $x=0$ .

$$W_1(0) = 0, W_1(1) = 0, W_2(0) = 0, W_2(1) = 0 \quad (24)$$

At  $x=L$ ;

$$\sum_{i=0}^{\infty} W_1(i) = 0, \sum_{i=0}^{\infty} i(i-1)W_1(i) = 0, \sum_{i=0}^{\infty} W_2(i) = 0, \sum_{i=0}^{\infty} i(i-1)W_2(i) = 0 \quad (25)$$

By assuming  $W_1(2) = c_1$ ,  $W_1(3) = c_2$ ,  $W_2(2) = c_3$ ,  $W_2(3) = c_4$  the Eqs. (14) and (15) can be calculated up to  $n$  terms and a similar procedure is followed as that of simply supported boundary condition.

## 4. Results and Discussion

### 4.1. Comparison with analytical solution

In this study, we consider double-walled carbon nanotubes embedded in an elastic (Winkler) medium having the inner and outer diameters of 0.7 nm and 1.4 nm, respectively. The effective thickness of each nanotube is taken to be that of graphite sheet with 0.34 nm. The carbon nanotube has an elastic modulus of 1TPa and the density of 2.3 gm/cm<sup>3</sup> [17, 19].

By using the differential transformation method as the numerical method, the natural frequency for double-walled carbon nanotubes embedded in an elastic medium has been computed. Results are compared with Elishakoff and Pentaras [17] study in which they used Buvnov-Galerkin, and Petrov-Galerkin methods for analysing vibration response of double-walled carbon nanotubes. Also, results are

compared with Xu et al. [20] study in which they used the exact method to find the vibration responses of double-walled carbon nanotubes embedded in an elastic medium. Comparison results are shown in Tables 3, 4, and 5.

Very good agreement is observed with the exact solutions for simply supported boundary condition as of Elishakoff and Pentaras [17]. Again, good agreement with Bubnov method of Elishakoff and Pentaras [17] and Xu et al. [20] results are demonstrated. We have taken  $n=45$  so that the result converges up to four decimal places. Where  $n$  is the number of iterations.

Clearly, it is observed that Fundamental frequency of double-walled carbon nanotubes decreasing with increasing aspect ratio  $L/d$ , where  $d$ =diameter of outer nanotube.

**Table 3. Simply supported DWCNTs fundamental frequency in THz.**

$L/d$	10	12	14	16	18	20
Present [DTM]	0.46830	0.32527	0.23899	0.18298	0.14467	0.11716
Exact [17]	0.46830	0.32527	0.23899	0.18298	0.14467	0.11716
Bubnov [17]	0.47211	0.32791	0.24093	0.18447	0.14576	0.11806
Petrov [17]	0.46884	0.32564	0.23926	0.18319	0.14475	0.11725
Xu et al. [20]	0.46	.....	.....	.....	.....	0.11

**Table 4. 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 [17]	1.07986	0.75063	0.55171	0.42248	0.33385	0.27043
Petrov [17]	1.06478	0.73087	0.54341	0.41135	0.32505	0.26331
Xu et al. [20]	1.06367	.....	.....	.....	.....	0.2660

**Table 5. Clamped-hinged DWCNTs fundamental frequency in THz.**

$L/d$	10	12	14	16	18	20
Present [DTM]	0.73140	0.50857	0.37288	0.28583	0.22585	0.18294
Bubnov [17]	0.73277	0.50909	0.37409	0.28644	0.22634	0.18334
Petrov [17]	0.72843	0.50607	0.37188	0.28474	0.22499	0.18225
Xu et al. [20]	0.728	.....	.....	.....	.....	0.1834

#### 4.2. Influence of surrounding medium on vibration frequencies of double-walled carbon nanotubes (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 listed in Figs. 2 to 4.

It is observed that vibration frequencies of first in-phase modes are highly influenced by the Winkler elastic medium.



From Figs. 2, 3, and 4, 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. On the other hand, stiffness of surrounding medium impacts little on the vibration frequencies of the antiphase modes. Results for the first six modes have been demonstrated.

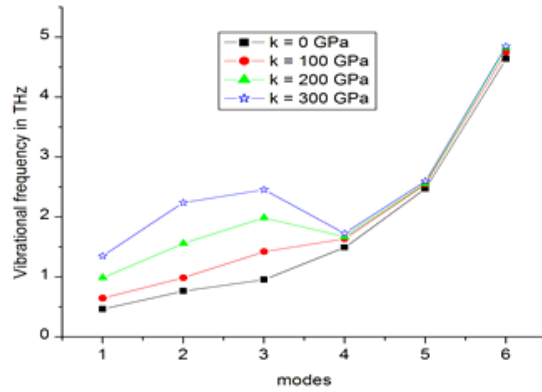


Fig. 2. Vibration frequencies for simply-supported DWCNTs.

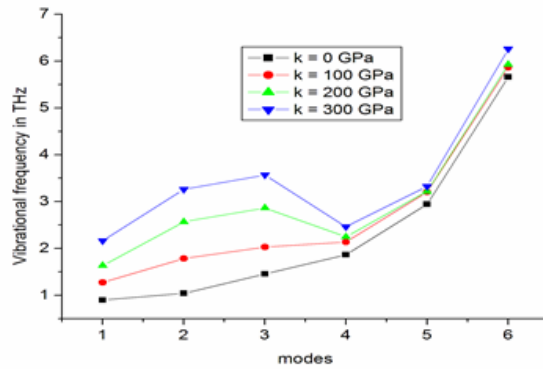


Fig. 3. Vibration frequencies for clamped-clamped DWCNTs.

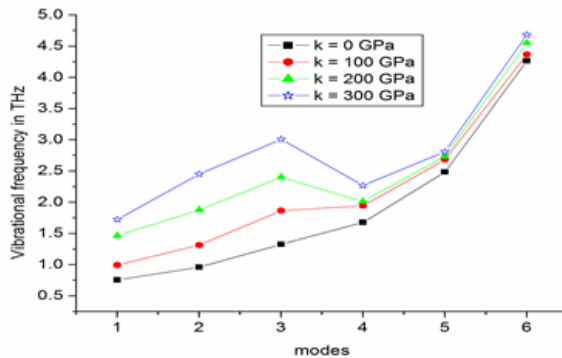


Fig.4. Vibration frequencies for clamped – Hinged DWCNTs.

## 5. Conclusions

In this study, the vibration analysis of double-walled carbon nanotubes embedded in an elastic medium for various boundary conditions like clamped-clamped, simply supported, and clamped hinged are studied by a semi-analytical numerical technique called the Differential transform method in a simple and accurate way. The solution of the present vibration analysis problem using the differential transformation method includes transforming the governing equations of motion into algebraic equations and solving the transformed equations. Some concluding observations from the investigation are given below.

- Fundamental frequency decreases with increasing aspect ratio ( $L/d$ ).
- Results indicate that phase modes have a strong influence on vibration frequencies of carbon nanotubes.
- The stiffness of surrounding medium affects the resonant frequencies of double-walled carbon nanotubes, especially for the first in-phase modes.
- On the other hand, the stiffness of the surrounding medium impacts little on the resonant frequencies of the antiphase modes.

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