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Vibration response of double-walled carbon nanotubes embedded in an elastic medium with inter-tube Vander waals forces

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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. In this work differential transform method(DTM) is used to study the vibrational behavior of the double walled carbon nanotubes(DWCNT) for various boundary conditions. Elastic continuum models are used to study the vibrational behavior of CNTs 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 embedded in an elastic medium, a theoretical analysis is presented based on Euler-Bernoulli beam model and Winkler spring model.
Keywords : *Aerospace , Buvnov-Galerkin, DTM, DWCNT, MATLAB, Petrov-Galerkin.*

Introduction

Iijima's discovery paper on multi-walled carbon nanotubes in 1991 [1] led to a major revolution in the area of nanoscience and nanotechnology. Carbon nanotubes (CNTs) 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 need for new materials which exhibit improved mechanical properties i.e, high strength at reduced weight. Carbon nanotubes (CNTs) are allotropes of carbon with a cylindrical nanostructure. Nanotubes have been constructed with length-to-diameter ratio of up to 132,000,000:1[2], significantly larger than any other material. The structure of an SWCNT can be conceptualized by wrapping a one-atom-thick layer of graphite called graphene into a seamless cylinder [2], [3] and [6]. Single-walled nanotubes are the most likely candidate for miniaturizing electronics beyond the micro-electromechanical scale currently used in electronics [9]. Single-walled nanotubes are an important variety of carbon nanotube because they exhibit electric properties that are not shared by the multi-walled carbon nanotube (MWNT) variants[2].Carbon nanotubes are the strongest and stiffest materials yet discovered in terms of tensile strength and Elastic Modulus respectively[7]. Since carbon nanotubes have a low density for a solid of 1.3 to 1.4 $g{\cdot}cm^{-3}$[13]. This strength results from the covalent sp^2 bonds formed between the individual carbon atoms.

size-dependent continuum-based methods [5–7] are becoming popular in modeling small sized structures as it offers much faster and accurate solutions. Sudak [8] carried out buckling analysis of multi-walled carbon nanotubes. Wang and Varadhan [9] analyzed the small scale effect of CNT and shell model. Yakobson et al. [10] introduced an atomistic model for axially compressed SWCNT and compared it to a simple continuum shell model. Sears and Batra[11] proposed a comprehensive buckling analysis of single walled and multi-walled CNTs by molecular mechanics simulations and continuum mechanics models.

In the present work, DTM has been used to study the vibration of CNTs embedded in an elastic medium. Zhou [16] proposed differential transformation method to solve both linear and non-linear initial value problems in electric circuit analysis. Later Chen and Ho [17] applied this method to eigen value problems. Arikoglu and ozkol [18] applied differential transformation method to solve the intergro – differential equation.

Differential Transform Method:

The Differential transform method is a semi-analytical method based on the Taylor series expansion. In this method, certain transformation rules are applied and the governing differential equations and the boundary conditions of the system are transformed into a set of algebraic equations in terms of the differential transforms of the original functions. The solution of these algebraic equations gives the desired solution of the problem.

The differential transformation of the kth derivative of the function u(x) is defined as follows:

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

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

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

In real application function, u(x) is expressed as finite series and equation (2) can be written as:

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

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.

Table 1: Differential Transformations for Mathematical Equations

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

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 [18]

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

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

For the DWCNTs, the interaction between inner and outer nanotubes is considered to be coupled together through the Vander Waals (vdW) forces. Equation (4) can be used to each layer of the inner and outer nanotubes of the DWCNTs. Assuming that the inner and outer tubes have the same thickness and effective material constants. Based on the Euler-Bernoulli beam model, we have:-

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

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

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.

The pressure P_1 acting on the inner nanotube caused by vdW interaction is given by

$$p_1 = c(w_2 - w_1) \quad (7)$$

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

Fig.1 shows the analysis model CNTs embedded in an elastic medium. The pressure acting on the outermost layer due to the surrounding elastic medium can be given by

$$p_w = -kw_2 \quad (8)$$

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

Thus, for the embedded DWCNTs, the pressure of the outermost nanotube contacting with the elastic medium is given by

$$p_2 = p_w - c(w_2 - w_1) \quad (9)$$

In the simulation vdW interaction coefficient (c) can be obtained from the interlayer energy potential, given as [13]

$$c = \frac{320 \times (2R1) erg / cm^2}{0.16 d^2}, d = 0.142 nm \quad (10)$$

where,

R1= Radius of the inner nanotube.

Thus,

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

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

In this analysis, we consider the deflection of DWCNTs has different vibrational modes , $W_j(x)$, j = 1,2 for the inner and outer nanotubes. The displacements of the vibrational solution in DWCNTs can be given by

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

Which can be further simplified as:-

$$\frac{d^4\overline{W}_1}{dX^4} - \Omega^2\overline{W}_1 = \beta(\overline{W}_2 - \overline{W}_1) \tag{14}$$

$$(\delta).\frac{d^4\overline{W}_2}{dX^4} - \eta.\Omega^2\overline{W}_2 = \beta(\overline{W}_1 - \overline{W}_2) - \bar{k}.\overline{W_2} \tag{15}$$

Where,

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

Boundary Conditions:

A. Simply Supported CNT

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

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

B. Clamped-Clamped CNT

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

$$w_1 = 0, \frac{d\, w_1}{dx} = 0, w_2 = 0, \frac{d\, w_2}{dx} = 0 \tag{17}$$

C. Clamped-Hinged CNT

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

At x=0

$$w_1 = 0, \frac{d\, w_1}{dx} = 0, w_2 = 0, \frac{d\, w_2}{dx} = 0 \tag{18}$$

At x=L

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

Results and Discussions :

D. Comparision with Analytical Solutions

In this study, we consider double walled carbon nanotubes embedded in an elastic (Winkler) medium having the inner and outer diameters of 0.7nm and 1.4 nm, respectively. The effective thickness of each nanotube is taken to be that of graphite sheet with 0.34 nm. The CNT has an elastic modulus of 1 TPa and the density of 2.3 g / cm^3 [13,18].

By using the DTM as the numerical method the natural frequency for DWCNTs has been computed. Results are compared with Elishakoff & penataras et al [18] study in which he used Buvnov-Galerkin and Petrov-Galerkin methods for analyzing vibration response of DWCNTs. Also, Results are compared with Xu et al [26] and exact results. Very good agreement is observed with the exact solution. We have taken n= 50 so that the result converges up to four decimal places. Where n is the number of iterations required to converge the result.

Table 2: - Simply supported (S-S) DWCNTs Fundamental frequency in THz

L/d	**10**	**12**	**14**	**16**	**18**	**20**
Present[DTM]	0.4683	0.3252	0.2389	0.1829	0.1446	0.1171
Exact[18]	0.4683	0.3252	0.2389	0.1829	0.1446	0.1171
Bubnov[18]	0.4721	0.3279	0.24093	0.1844	0.1457	0.1180
Petrov [18]	0.4688	0.3256	0.2392	0.1831	0.1447	0.1172
Xu et al[26]	0.46	…….	…….	……..	……..	0.11

Table 3: - Clamped-Clamped (C-C) DWCNTs Fundamental Frequency in THz

L/d	**10**	**12**	**14**	**16**	**18**	**20**
Present[DTM]	1.0640	0.7368	0.5425	0.4137	0.3265	0.2654
Bubnov[18]	1.0798	0.7506	0.5517	0.4224	0.3338	0.2704
Petrov[18]	1.0647	0.7308	0.5434	0.4113	0.3250	0.2633
Xu et al[26]	1.0636	……	……	…….	…….	0.2660

Table 4: -Clamped-Hinged (C-H) DWCNTs Fundamental Frequency in THz

L/d	**10**	**12**	**14**	**16**	**18**	**20**
Present[DTM]	0.7314	0.5085	0.3728	0.2858	0.2258	0.1829
Buvnov[18]	0.7327	0.5090	0.3740	0.2864	0.2263	0.1833
Petrov[18]	0.7284	0.5060	0.3718	0.2847	0.2249	0.1822
Xu et al[26]	0.728	…….	…….	…….	……..	0.1834

Clearly it is observed that fundamental frequency of DWCNTs decreasing with increasing aspect ratio (L/d, where d=diameter of the outer nanotube) of nanotubes.

E. 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 given below.

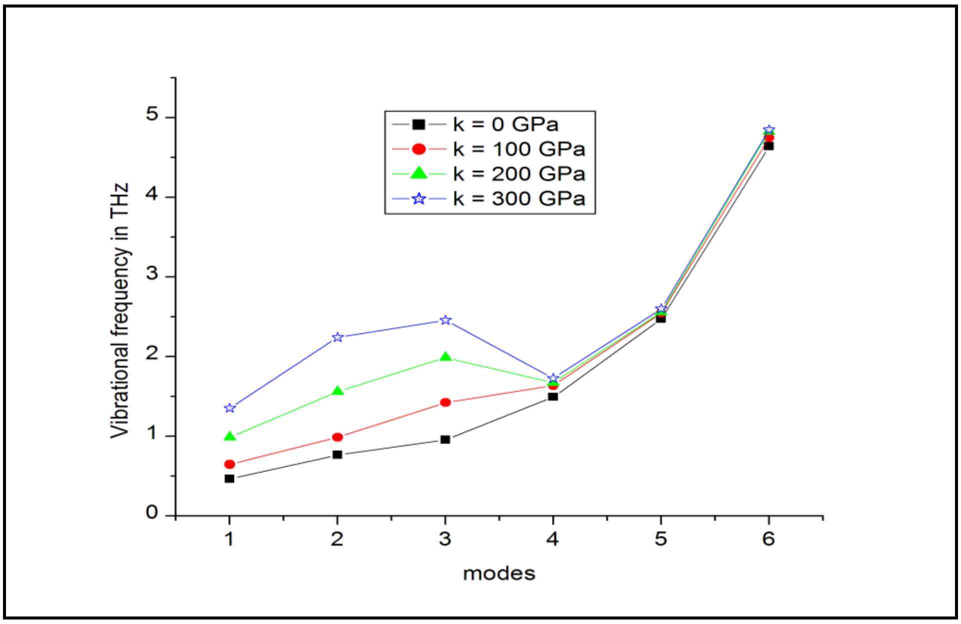

Fig 1: Influence of Winkler foundation on Vibration frequencies for simply supported DWCNTs

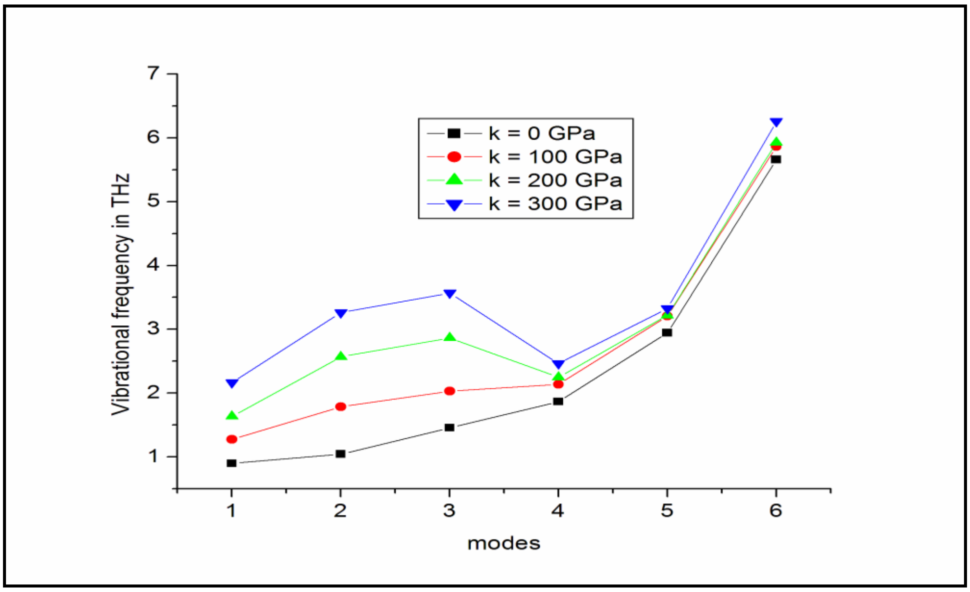

Fig 2: Influence of Winkler foundation on Vibration frequencies for Clamped-Clamped DWCNTs

Influence of the surrounding medium on the vibration frequency is investigated based on the Winkler spring model. It is found that vibration frequencies of the embedded double walled carbon nanotubes are larger than those of the nested 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 very little on the frequencies of the anti-phase modes.

Conclusion:

In this study, the vibration analysis of DWCNTs 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 DTM includes transforming the governing equations of motion into algebraic equations and solving the transformed equations. Results indicate that phase modes have a strong influence on vibration frequencies of CNTs. The stiffness of surrounding medium affects the resonant frequencies of DWCNTs, especially for the first in-phase modes. The investigation presented may be helpful in the application of CNTs such as high-frequency oscillators, dynamic mechanical analysis and mechanical sensors.

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