Elastic coupled vibrations in multi-walled carbon nanotubes

Julio R. Claeyssen, **Teresa Tsukzan**,
UFRGS - Instituto de Matemática-Promec
90.001-970, Porto Alegre, RS
E-mail: julio@mat.ufrgs.br, teresa@mat.ufrgs.br,

Rosemaira Dalcin Copetti
UFSM - Departamento de Matemática
97105-900, Santa Maria, RS
E-mail: rmaira@smail.ufsm.br

Resumo

Structural multi-span beams are considered with van der Waals interaction elastic forces in the modeling of multi-walled carbon nanotubes (MWNT). The eigenvalue problem is formulated in matrix form in terms of a new basis for all segments. This basis is generated by a fundamental matrix response.

1 Introduction

This work is about transverse responses in Euler-Bernoulli multi-span beams subject to interaction elastic forces in the modeling of multi-walled carbon nanotubes (MWNT).

Free vibrations of stepped beams have been studied by several authors by example [1-13], among others. In [13], a bi-segmented beam with a discontinuity in the cross-section and an intermediate device is studied. By keeping the original formulation of the physical problem, we face a non-classical quadratic eigenvalue problem depending upon frequency. This is accomplished by choosing a basis generated by a fundamental response and it derivatives, [15-17].

Carbon nanotubes (CNTs), discovered by Iijima [7], are cylindrical macromolecu1es composed of carbon atoms in a periodic hexagonal arrangement. As they are found, to have remarkable mechanical, physical, and chemical properties, carbon nanotubes hold exciting promise as structural elements in nanoscale devices or reinforcing element in superstrong nanocomposites. Typically, the nanotubes are about 2-15 nm in diameter and about 100-200 nm in length. They exhibit a Young modulus E of 1.2TPa and they support tensions several hundreds higher from those applied to iron. Nanotubes are thermally stable up to 2800^oC (in vacuum) and exhibit a thermal conductivity about twice as high as diamond [12], and may exhibit a capacity to carry electric current a thousand times better than cooper wires [4]. The importance in studying vibrations in CNTs is because of their mechanical and electronic properties in a number of nanomechanical devices such as oscillators, charge detectors, clocks, field emission devices and sensors. CNTs vibrations also occur during certain manufacturing processes (e.g., ultrasonication in nanocomposite processing) and as part of some nondestructive evaluation processes (e.g., Raman spectroscopy). lt is thus important to have accurate theoretical

models for the natural frequencies and mode shapes of carbon nanotubes for several reasons. Since controlled experiments at the nanometer scale are difficult with *wide scatter* in the experimental reported values, and molecular dynamics simulations remain formidable for large-scale systems ($10^6 - 10^8$ atoms for a few nanoseconds), continuum elastic models have been widely and successfully used to study mechanical behavior of CNT's, such as static deflection, thermal vibration, and resonant frequencies. In the analysis of one-dimensional beamlike structures, two models are usually employed, namely the Euler-Bernoulli and the Timoshenko beam model. For short beams, higher modes, and/or beam materials having E/G ratios (G shear modulus of the beam), the effects of through-thickness shear deformation and rotary inertia can be become significant, in which case the Timoshenko beam theory can be more accurate at the terahertz level. For double (DWNT) or multi-wall concentric nanotubes (MWNTs), the most widely used model in the literature assumes that all nested tubes of a MWNT remain coaxial during deformation and thus can be described by a single deflection model. However, this model can not be used to describe intertube relative vibration of MWNTs. It has been recently proposed by [15] that each nested concentric nanotube be considered as an individual beam, and the deflections of all nested tubes be coupled through the van der Waals interaction force between two adjacent tubes. The MWNT model to be considered in this work, will be then a set of N coupled Euler-Bernoulli equations coupled through the van der Walls interaction.

2 Structural and molecular mechanics

Due to the nature of the molecular force fields between two atoms, they can be treated as forces acting between two junctions (or material points) that are separated by structural beam or spring elements. Thus, the lattice of the carbon nanotubes can be considered as a three dimensional hexagonal network of beam (covalent) and spring (non-covalent) elements. The beam elements representing the bond are assumed to be isotropic with length L, cross-sectional area A, and moment of inertia I. According to the theory of classical structural mechanics, the strain energy of a uniform beam of length L subjected to pure axial force N, [9].

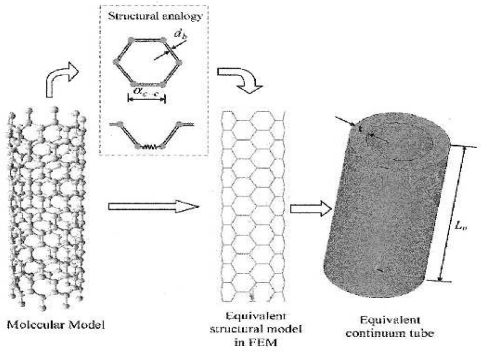


Figura 1: Equivalence of molecular, numeric and continuum models

A direct relationship between the structural mechanics parameters $EA, EI$and GJ and the molecular mechanics parameters $k_r,\ k_0$ and k_σ corresponding to the bond stretching force constant, bond angle bending force constante and torsional resistance, respectively, can be deduced [9] to be

$$\frac{EA}{L} = k_r, \quad \frac{EI}{L} = k_0, \quad \frac{GJ}{L} = k_\sigma, \quad (1)$$

Eq. (1) establishes the foundation of applying the theory of structural mechanics to the modeling of carbon nanotubes or other similar fullerene structures. As long as the force constants $k_r,\ k_0$ and k_σ are known, the sectional stiffness parameters EA, EI and GJ can be readily obtained. And then by following the

solution procedure of stiffness matrix method for frame structures, the deformation and related elastic behavior of graphene sheets and nanotubes at the atomistic scale can be simulated.

To calculate the effective properties of a nanotube based on a numerical method approach such as FEM it is assumed that the nanotube can be represented by an equivalent continuum tube shown in Fig. 1.

For real structures, the boundary conditions are always a challenge [6] mentions for nanostructures the situation be even more difficult. A cantilever beam assumption implies that one end is fixed but it may be necessary to include the elasticity at the support of such end. The vibration testing of composite beams and plates at the macromechanical level remains to be seen if it is appropriate at the nanomechanical level.

3 Multi-wall beam model for carbon nanotubes

A continuum approach using the well known frequency equation for a beam has been employed by several investigators to estimate the theoretical fundamental flexural resonance frequencies of nanotubes. For example, according to the well-known Bernoulli-Euler beam theory, the equation describing transverse, or flexural motion of a continuous, homogeneous, isotropic, linear elastic beam which without rotary inertia or shear effects and whose properties do not vary along its length may be expressed as

$$\rho A\frac{\partial^2 u(t,x)}{\partial t^2} + EI\frac{\partial^4 u(t,x)}{\partial x^4} = p(x) \qquad (2)$$

where x is the axial coordinate, t is time, p(x) is the transverse pressure per unit axial length, w is the deflection of the beam, I and A are the moment of inertia and the area of the cross section of the beam, and E and ρ are Young's modulus of beam material and the mass density. Thus, EI denotes the bending stiffness of the beam, and ρA represents the mass density per unit axial length.

It is known that multi-walled carbon nanotubes are distinguished from traditional elastic beams by their hollow multi-layer structure and associated intertube van der Waals forces. The equation (2) can be used to each of the inner and outer tubes of the multi-walled carbon nanotubes. Assuming that the inner outer tubes have the same thickness and effective material constants, that deflection linear vibration are small, the van der Waals pressure at any point between the tubes should be a linear function of the jump in deflection at that point.Thus the interaction pressure per unit axial length is given by $p = c(u_2 - u_1)$, [16], where u_1 e u_2 are the deflections in the inner and outer nanotubes, respectively, and the interaction coefficient per unit length between any two adjacent layer c, can be estimated by

$$c_j = \frac{\alpha(2R_j)erg/cm^2}{0.16d^2} \quad (d = 0.142nm), \qquad (3)$$

where R_j is the radius of the j-th tube, and the constant $\alpha = 320$ in [16], $\alpha = 400$ in [1].

The multiple-elastic beam model for N-walled carbon nanotubes (CNT), based on the Euler-Bernoulli beam theory, is governed by the following set of N-coupled equations [21]

$$\begin{aligned}
&\rho A_1\tfrac{\partial^2 u_1(t,x)}{\partial t^2} + EI_1\tfrac{\partial^4 u_1(t,x)}{\partial x^4} + c_1(u_1 - u_2) = 0,\\
&\vdots\\
&\rho A_j\tfrac{\partial^2 u_j(t,x)}{\partial t^2} + EI_j\tfrac{\partial^4 u_j(t,x)}{\partial x^4} +\\
&\qquad +c_j(u_j - u_{j+1}) - c_{j-1}(u_{j-1} - u_j) = 0,\\
&\qquad\qquad\qquad\qquad j = 2,3,..,N-1,\\
&\vdots\\
&\rho A_N\tfrac{\partial^2 u_N(t,x)}{\partial t^2} + EI_N\tfrac{\partial^4 u_N(t,x)}{\partial x^4} +\\
&\qquad\qquad\qquad +c_{N-1}(u_N - u_{N-1}) = 0.
\end{aligned}$$

where x is axial coordinate of the beam, $u_j(t,x)$ the deflexion of the $j-th$ CNT, I_j and A_j the moment of inertia and the area of the

cross-section of the $j-th$ tube, E is the Young´s modulus and ρ the mass density (E=1 TPa, $\rho = 1.3gr/cm^3$).

This coupled model can be written in matrix form as

$$M\frac{\partial^2 u}{\partial t^2} + K\frac{\partial^4 u}{\partial x^4} + Cu = 0, \tag{4}$$

where $M = diag[\rho A_1, \cdots, \rho A_N]$, $K = diag[EI_1, \cdots, EI_N]$,, $u = col[u_1 \cdots u_N]$ and C is the matrix

$$\begin{bmatrix} c_1 & -c_1 & \cdots & 0 & 0 \\ -c_1 & (c_2+c_1) & \cdots & 0 & 0 \\ \cdot & \cdot & \cdot & 0 & \cdot \\ 0 & 0 & \cdots & (c_{N-2}+c_{N-1}) & -c_{N-1} \\ 0 & 0 & \cdots & -c_{N-1} & c_{N-1} \end{bmatrix}.$$

4 Free transverse vibrations

The solution of system of homogeneous matrix partial differential equations (4) can be written in terms of a vector exponential

$$u(t,x) = e^{t\lambda}U(x). \tag{5}$$

where $U = col[U_1 U_2 \cdots U_N]$. Substituting the solution in (4), we have that $U(x)$ satisfies the fourth-order differential equation with matrix coefficients

$$KU^{iv}(x) + (\lambda^2 M + C)U(x) = 0. \tag{6}$$

Since K is not singular, we can write the above equation as

$$U^{(iv)}(x) + AU(x) = 0. \tag{7}$$

where $A = K^{-1}(\lambda^2 M + C)$. In the study of wave propagation, it is considered the harmonic wave amplitude $U(x) = e^{ikx}v$ and natural frequencies, that is, $\lambda = i\omega$. This will lead to

$$\left[k^4 K + (-\omega^2 M + C)\right] v = 0, \tag{8}$$

This generalized eigenvalue problem can be solved by numerical methods for frequencies ω or wavenumbers k. See [11] for simulations by using the power method or by Krylov method.

With beams of finite length, generic spatial boundary conditions of classical or non-classical nature can be written as

$$\begin{aligned} &A_{11}U_1(0) + B_{11}U_1'(0) + C_{11}U_1''(0) + D_{11}U_1'''(0) = 0, \\ &A_{12}U_1(0) + B_{12}U_1'(0) + C_{12}U_1''(0) + D_{12}U_1'''(0) = 0, \\ &A_{21}U_N(L) + B_{21}U_N'(L) + C_{21}U_N''(L) + D_{21}U_N'''(L) = 0, \\ &A_{22}U_N(L) + B_{22}U_N'(L) + C_{22}U_N''(L) + D_{22}U_N'''(L) = 0. \end{aligned}$$

In the case of non-classical boundary conditions, the coefficients might depend upon frequency λ. For instance, for a cantilever beam (clamped-free) we have

$$\begin{aligned} U_1(0) = 0, \quad U_1'(0) = 0, \\ U_N''(L) = 0, \quad U_N'''(L) = 0, \end{aligned} \tag{9}$$

while for a torsional spring of rotational constant σ restrained and free end beam, we have

$$\begin{aligned} EI_1 U_1''(0) + \sigma U_1'(0) = 0, \quad U_1'''(0) = 0 \\ U_N''(L) = 0, \quad U_N'''(L) = 0. \end{aligned} \tag{10}$$

If a mass m is attached at the free end of a clamped beam, we shall have

$$\begin{aligned} U_1(0) = 0, \qquad\qquad U_1'(0) = 0, \\ U_N''(L) = 0, \quad EI_N U_N'''(L) - m\lambda^2 U_N(L) = 0. \end{aligned}$$

The last condition corresponds to the equilibrium between inertia force and shear force. Since inertia force is associated with the acceleration of the body, this will induce the quadratic term in λ.

General conditions of continuity or compatibility for the displacement U_j, the slope U_j', the bending moment $EI_j U_j''$ or for the jump in the internal shear force $EI_j U_j'''$ when there is an applied force or a physical device at an intermediate location or a simply discontinuity in the transversal section at the point x_j, $j = 1, 2, .., N-1$ can be written as

$$\begin{aligned} &U_j(x_j) = U_{j+1}(x_j), \;\; U_j'(x_j) = U_{j+1}'(x_j), \\ &EI_j U_j''(x_j) = EI_{j+1} U_{j+1}''(x_j), \\ &EI_j U_j'''(x_j) = EI_{j+1} U_{j+1}'''(x_j) + F_j, \end{aligned} \tag{11}$$

where F_j denotes the force exerted by the intermediate device. These equations include the case of an intermediate support at x_j. We simple consider the first two equations for zero displacement at x_j^+ and x_j^-. Then the continuity of the rotation or inertia moment and for the bending moment at a x_j^+ and x_j^-. For the case of a torsional spring or a rotational mass, the bending moment has a jump at an intermediate support [6].

4.1 Matrix basis

The general solution of (7) can be written [2] as

$$U(x) = \mathbf{h}(x)c_1 + \mathbf{h}_1'(x)c_2 + \mathbf{h}''(x)c_3 + \mathbf{h}'''(x)c_4 \tag{12}$$

for arbitrary vectors c_1, c_2, c_3 and c_4 de order $n \times 1$. Here $\mathbf{h}(x)$ is the solution of the initial value problem $\mathbf{h}^{(iv)}(x) + A\mathbf{h}(x) = 0$ subject to the initial conditions $\mathbf{h}(0) = 0$, $\mathbf{h}'(0) = 0$, $\mathbf{h}''(0) = 0$, $\mathbf{h}'''(0) = I$ where 0 denotes the $N \times N$ null matrix and I the $N \times N$ identity matrix. This solution is said referred to as the *fundamental matrix response*. For determining $\mathbf{h}(x)$, we first consider the characteristic polynomial

$$P(s) = det[s^4 I + A] = \sum_{k=0}^{4N} b_k s^{4N-k}.$$

Then we find the solution $h(x)$ of the initial value problem

$$\begin{array}{l} \sum_{k=0}^{4N} b_k h^{(4N-k)}(x) = 0. \\ h(0) = h'(0) = \cdots = h^{(4N-2)}(0) = 0, \\ b_0 h^{(4N-1)}(0) = 1 \end{array}$$

and we let $\mathbf{h}_k$ be the solution of the matrix difference equation

$$\begin{array}{l} \mathbf{h}_{k+4} + A\mathbf{h}_k = 0 \\ \mathbf{h}_o = 0, \mathbf{h}_1 = 0, \mathbf{h}_2 = 0, \mathbf{h}_3 = I. \end{array} \tag{13}$$

We have

$$\mathbf{h}(x) = \sum_{j=1}^{4N} \sum_{i=0}^{j-1} b_i h^{(j-1-i)}(x) \mathbf{h}_{4N-j} \tag{14}$$

A normalized basis [2], could also be used.

4.2 The case of a double layer carbon nanotube

For a double layer carbon nanotube, we have the matrix coefficients

$$M = \begin{bmatrix} m_1 & 0 \\ 0 & m_2 \end{bmatrix} \quad , \quad C = \begin{bmatrix} c_1 & -c_1 \\ -c_1 & c_2 \end{bmatrix},$$
$$K = \begin{bmatrix} k_1 & 0 \\ 0 & k_2 \end{bmatrix}$$

The characteristic polynomial is given by

$$P(s) = \alpha s^8 + \beta^4 s^4 + \theta \tag{15}$$

where

$$\alpha = E^2 \, II_1 \, II_2, \tag{16}$$

$$\beta = \frac{II_1 \, \lambda^2 \, \rho \, A_2 + II_1 \, c_2 + \lambda^2 \, \rho \, A_1 \, II_2 + c_1 \, II_2}{E \, II_1 \, II_2}$$

$$\theta = \frac{\lambda^4 \, \rho^2 \, A_1 \, A_2 + \lambda^2 \, \rho \, A_1 \, c_2 + c_1 \, \lambda^2 \, \rho \, A_2 + c_1 \, c_2 - 1. \, {c_1}^2}{E^2 \, II_1 \, II_2}$$

The roots of this polynomial are of the type $r_1 = \epsilon$; $r_2 = -\epsilon$; $r_3 = i\epsilon$; $r_4 = -i\epsilon$; $s_1 = \delta$; $s_2 = -\delta$; $s_3 = i\delta$; $s_4 = -i\delta$, where ϵ and δ depend upon the eigenvalue λ. It turns out that

$$d(x) = \frac{\sinh(\varepsilon \, t) - \sin(\varepsilon \, t)}{8 \, \varepsilon^7 + 4 \, \beta \, \varepsilon^3} + \frac{\sinh(\delta \, t) - \sin(\delta \, t)}{8 \, \delta^7 + 4 \, \beta \, \delta^3}$$

By iterating (13) and substituting values, we obtain that $h(x)$ is given by the symmetric matrix EDF

$$h(x) = \begin{bmatrix} a_1 d(x) + k_2 d^{(iv)}(x) & -c_1 d(x) \\ -c_1 d(x) & a_2 d(x) + b_2 d^{(iv)}(x) \end{bmatrix}$$

where

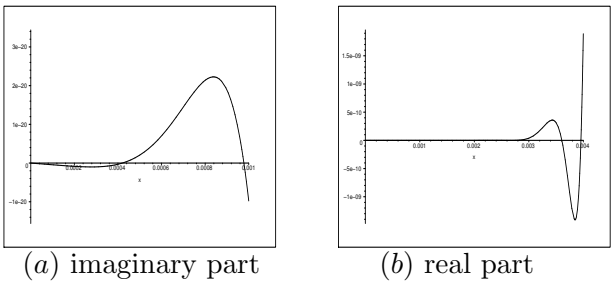
$$a_1 = \frac{(2 \, c_1 \, k_2 + k_1 \, \lambda^2 \, m_2 + k_1 \, c_2) \, d}{k_1},$$
$$a_2 = \frac{(2 \, k_1 \, c_2 + \lambda^2 \, m_1 \, k_2 + c_1 \, k_2) \, d}{k_2}$$

and $b_1 = k_2$, $b_2 = k_1$.

4.3 Characteristic Equation

The characteristic equation for finding the modes $\mathbf{U}(x)$ will amount to find a solution of (7) that satisfies the boundary or compatibility conditions. Since the general solution (12) depend upon 4N constants and we have 4 boundary conditions and 4(N-1) compatibility conditions, the problem that will result in terms of $\mathbf{h}$ and its derivative at intermediate and end points of the beam and the coefficients c_1, c_2, c_3, c_4, will set up a homogeneous algebraic system. The existence of non-zero solutions will give us the characteristic equation for the problem. Eventually, the determination of the constants might be simplified by using a similar technique on the one developed in the physical space, rather that using a state formulation. Our approach is more appropriate and general than Yoon, [15]. He assumed that the components of an oscillating mode differ only by constants. This artifice allowed him to decouple the stationary system and to refer things in a simpler manner with a single fourth-order differential equation. We observe that for the data considered by Yoon, [15] the basic function $d(x)$ turns out to be in general a complex one. Thus pure oscillations and real vibrations might exist when a parameter is varied. This is the case in the terahertz level where complex oscillations collapse into a simple real oscillation.

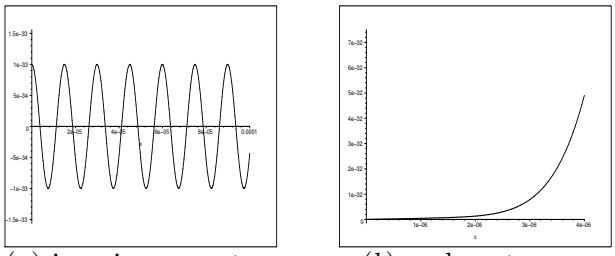
5 Simulations



(a) imaginary part (b) real part

Figura 2: Eigenfunction at $\lambda = 4.73X10^{(-9)}$

Here we illustrate the bifurcation phenomena at the terahertz level for a double wall carbon nanotube.



(a) imaginary part (b) real part

Figura 3: Eigenfunction λ=5.38I terahertz

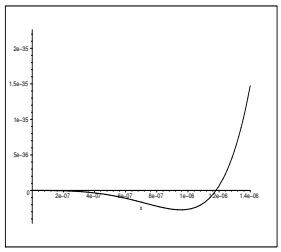


Figura 4: Eigenfunction λ= 6.0I terahertz

6 Concluding remarks

A continuum approach using the well known frequency equation for a beam has been employed by several investigators to estimate the theoretical fundamental flexural resonance frequencies of nanotubes. Here the frequency equation and the modal system of multi-span Euler-Bernoulli coupled beams with discontinuous cross-section have been formulated in terms of the dynamical basis generated by the fundamental solution $h(x)$ of a coupled fourth-order matrix differential equation. This later accounts for the interaction forces in the nanotubes. The modes are then determined in a systematic manner in terms of $h(x)$ and its derivatives. This methodology can be applied to other kinds of beams that result from diverse approximations such as Rayleigh, shear beams or Timoshenko beams.

Referências

[1] A. Chakraboty, M. S. Sivakumur, S, Gopalakrishnan, "Spectral element based model for wave propagation analysis in multi-wall carbon nanotubes", Int. J. Solids and Structures, Vol. 43, pp. 279-294, 2006.

[2] J. R. Claeyssen, G. C. Suazo, C. Jung, "A Direct Approach to Second-Order Matrix Non-Classical Vibrating Equations Applied Numerical Mathematics", Journal of Sound and Vibration, Vol. 39, pp. 65-78, 1999.

[3] J. R. Claeyssen, S. N. J. Costa, "Modes for the coupled Timoshenko model with a restrained end", Journal of Sound and Vibration, Vol. 296, pp. 1053-1058, 2006.

[4] P. G. Collins, P. Avouris, "Nanotubes for electronics", Scientific American, Vol. 283(6), pp. 67-69, 2000.

[5] R. D. Copetti, J. R. Claeyssen, T. Tsukasan, "Free vibrations in Euler-Bernoulli multi-span beams with interaction forces in carbon nanotubes continuum", Proceedings of Dincon 2007, Brazillian Conference em Dynamics, Control and their Applications, São José do Rio Preto, São Paulo, 2007.

[6] R. F. Gibson, E. O. Ayorinde, Y. F. Wen, "Vibrations of carbon nanotubes and their composites: A review", Composites Science and Technology, Vol. 67, N 1, pp. 1-28, 2007.

[7] S. Iijima, "Helical microtubules of graphitic carbon", Nature, Vol. 354, pp. 1-8, 1991.

[8] A. L. Kalamkarov, A. V. Georgiades, S. K. Rokkam, V. P. Veedu, M. N. Ghasemi-Nejhad, "Analytical and numerical techniques to predict carbon nanotubes properties", Int. J. Solids and structures, Vol. 43, pp. 6832-6854, 2006.

[9] C. Li, T. W. Chou, "A structural mechanics approach for the analysis of carbon nanotubes", International Journal of Solids and Structures, Vol. 40, pp. 2487-2499, 2003.

[10] T. Natsuki, M. Endo, "Vibration analysis of embedded carbon nanotubes using wave propagation approach", Journal of Applied Physics, Vol. 99, pp. 034311, 2006.

[11] M. Scotti. O problema quadrático de autovalor em vibrações e nanotecnologia. Dissertação de Mestrado - UFRGS - 2006.

[12] E. T. Thostenson, Z. Ren, T. W. Chou, "Advances in the science and technology of carbon nanotubes and their composites: a review", Composites Science and Tecnology, Vol. 61, pp. 1899-1912, 2001.

[13] T. Tsukazan, "The Use of a Dynamical Basis for Computing the Modes of a Beam System with a Discontinuous Cross-Section", Journal of Sound and Vibration, Vol. 281, pp. 1175-1185, 2005.

[14] A. Uściłowska, J. A. Kołodziej, "Free vibrations of immersed column carrying a tip Mass", Journal of Sound and Vibration, Vol. 216(1), pp. 147-157, 1998.

[15] J. Yoon, C. Q. Ru, A. Miuduchowski, "Vibration of an embedded multiwwall carbon nanotube", Composites Science and Technology, VoL. 63, pp. 1533-1542, 2003.

[16] Y. Q. Zhang, G. R. Liu, X. Y. Xie, "Free transverse vibrations of double-walled carbon nanotubes using a theory of nonlocal elasticity", Physical Review B, VoL. 71, 195404, 2005.