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Dynamic stability of carbon nanotubes

Andrzej Tylikowski
Warsaw University of Technology, Institute of Machine Design Fundamentals
Narbutta 84, 02-524 Warszawa, Poland
aty@simr.pw.edu.pl

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The dynamical stability of carbon nanotubes embedded in an elastic matrix under time-dependent axial loading is studied in this paper. Effects of van der Waals interaction forces between the inner and outer walls of nanotubes are taken into account. Using continuum mechanics an elastic beam model is applied to solve the transverse parametric vibrations of two co-axial carbon nanotubes. The physically realizable forces with known probability distributions and uniformly distributed on the both beam edges are assumed as the tube axial loadings. The energy-like functionals are used in the stability analysis. The emphasis is placed on a qualitative analysis of dynamic stability problem. Influence of constant component of axial forces on stability regions is shown. Boundaries of dynamic stability regions are determined using the three models and techniques with different degree of accuracy.

Keywords: parametric vibration, dynamic stability of shells, carbon nanotubes, Liapunov method

1. Introduction

Due to novel electronic properties and high mechanical strength, carbon nanotubes have become promising materials for nanoelectronics, nanodevices, nanocomposites and nanomachines. Bending and elastic buckling of single- and multi-walled nanotubes have been object of numerous experimental, theoretical and molecular–dynamics simulations [1]. The results of atomic modeling for axially compressed single - walled nanotubes were compared with the results for elastic cylindrical shell models [9]. To apply the elastic shell model to carbon nanotubes, a most crucial point is to define the representative thickness of single-walled nanotubes. The representative thickness was assumed as the equilibrium interlayer spacing of adjacent nanotubes [3]. In many applications it has been tacitly assumed that the bending stiffness of nanotubes is given by the classic cylindrical bending stiffnes. In [5] the effective bending stiffness of single-walled nanotubes was introduced as an independent material parameter not related to the representative thickness by the classic bending stiffness formula. More recently, considerable attention has turned to mechanical behaviour of a single or multi-walled carbon nanotubes embedded in a plastic or metallic matrix. From the viewpoint of continuum modeling, carbon nanotubes are distinguish from classical elastic cylindrical shells due to their multi-walled structure and intertube van deer Waals forces [7]. Multi-walled nanotubes can be used as frictionless nano-actuators, nano-bearings, and nano-springs. The applicability of the cylindrical shell and beam models in the carbon nanotube buckling was explored and the benchmark was developed [10]. The research on static stability analysis of carbon nanotubes was performed via elastic continuum beam and shell models [8]. The actual applicability of the elastic cylindrical shell and beam model was discussed for different buckling phenomena of carbon nanotubes under different constant compressive loads. The simulations were validated by the existing experimental results or results obtained with molecular modeling. Recently, double-walled carbon nanotube oscillators of various lengths and construction were compared for their dissipation energy mechanisms under motion – induced self-heating [11]. The role of interlayer radial displacements in transverse vibrations of multi-walled nanotubes based on a simple linear model of multiple Euler beams [10] was studied. The thin-walled composite beams are subjected to a flattening effect leading to the strongly nonlinear equations [6]. The parametric vibrations dynamical stability of carbon nanotubes embedded in an elastic matrix under time-dependent axial loading is studied in this paper. Effects of van der Waals interaction forces between the inner and outer walls of nanotubes are taken into account [4]. Using continuum mechanics the multiple beam model is applied to solve the dynamic stability problem of transverse parametric vibrations of co-axial carbon nanotubes. The physically realizable forces with known probability distributions are assumed as the tube axial loading. The influence of constant component of axial force is also taken into account. The energy-like functionals are used in the stability analysis. The emphasis is placed on a qualitative analysis of dynamic stability problem. Boundaries of dynamic stability regions are determined using the two models and techniques with different degree of accuracy.

2. Thin-walled double co-axial beam model

Beam transverse displacements are denoted by w and u. Assuming the viscous damping, the linearized van der Walls interaction between tubes characterized by the coefficient c and the external nanotube-matrix interaction with constant d we obtain the coupled system of partial differential equations. The dynamic equations have the form

$$w_{,tt} + 2\beta w_{,t} + e w_{,xxxx} + \left(N_o + \tilde{N}\left(t\right)\right) w_{,xx} + c\left(w - u\right) = 0 \tag{1}$$

$$x \in (0, l)$$

$$u_{,tt} + 2\beta u_{,t} + e u_{,xxxx} + \left(N_o + \tilde{N}\left(t\right)\right) u_{,xx} + c\left(u - w\right) + du = 0 \tag{2}$$

$\tilde{N}\left(t\right)$ is the time-dependent component of axial force, $e = D/\rho A$, D is the tube effective bending stiffness, ρA is the mass of unit length and it is assumed that the radii of double-walled carbon nanotubes differ negligibly, β is the damping coefficient responsible for energy dissipation [11]. The both nanotubes are assumed to be simply supported at $x = 0$ and $x = l$ where the transverse displacements and bending moments are equal to zero

$$w(0,t) = w(l,t) = u(0,t) = u(l,t) = 0 \tag{3}$$

$$w_{,xx}(0,t) = w_{,xx}(l,t) = u(0,t) = u(l,t) = 0 \tag{4}$$

3. Dynamic stability analysis of the double beam model

Assume that the axial forces are physically realizable and it is known their probability distributions. In order to investigate almost sure dynamic stability of trivial solutions of equations (3) and (4) $w = u = 0$ we generate the Liapunov functional as a modification of the full shell energy. Assume that the axial forces acting in both thin-walled beams are equal and are uniformly distributed on the beams edges. In order to investigate almost sure dynamic stability of trivial solutions of equations (1) and (2) the Liapunov functional is taken in the form

$$\begin{gathered} V = \tfrac{1}{2}\int_0^l \left[w_{,t}^2 + 2\beta w_{,t}^2 + 2\beta^2 w^2 + u_{,t}^2 + 2\beta u_{,t}u + 2\beta^2 u^2 + e w_{,xx}^2 + \right. \\ \left. + e u_{,xx}^2 - N_o w_{,x}^2 - N_o u_{,x}^2 + c\,(w-u)^2 + du^2\right] dx \end{gathered} \tag{5}$$

It should be emphasized that functional (5) is positive definite, if the constant component of axial force N_o is smaller than Euler's critical force $e\,(\pi/l)^2$.

Due to the physical realizability it is possible to calculate the time derivative of functional (5) in a classical way

$$\begin{gathered} \tfrac{dV}{dt} = \int_0^l \left[w_{,t}w_{,tt} + \beta w w_{,tt} + \beta w_{,t}^2 + 2\beta^2 w w_{,t} + u_{,t}u_{,tt} + \beta u u_{,tt} + \right. \\ + \beta u_{,t}^2 + 2\beta^2 u u_{,t} + e w_{,xx} w_{,xxt} + e u_{,xx} u_{,xxt} + \\ \left. - N_o w_{,x} w_{,xt} - N_o u_{,x} u_{,xt} + (w-u)(w_{,t} - u_{,t})\, d u u_{,t}\right]\ dt \end{gathered} \tag{6}$$

Substituting the accelerations w and u from equations (1) and (2) respectively, and integrating by parts using the zero boundary conditions (3) and (4) we can simplify the time-derivative of functional. As an example the ninth component of the integrand is transformed in the following way

$$\int_0^l e w_{,xx} w_{,xxt} dx = e w_{,xx} w_{,xt}\Big|_0^l - \int_0^l e w_{,xxx} w_{,xt} dx = -e w_{,xxx}\ w_{,t}\Big|_0^l + \int_0^l e w_{,xxxx} w_{,t} dx \tag{7}$$

Using the technique presented in formula (7) we have

$$\frac{dV}{dt} = -2\beta V + 2U \tag{8}$$

where the auxiliary functional has the form

$$\begin{gathered} U = \tfrac{1}{2}\int_0^l \left[2\beta^2 w_{,t}^2 + 2\beta^3 w^2 + 2\beta^2 u_{,t} u + 2\beta^3 u^2 + \right. \\ \left. + \tilde{N}(t)\,(w_{,t} + \beta w)\, w_{,xx} + \tilde{N}(t)\,(u_{,t} + \beta u)\, u_{,xx}\right]\ dx \end{gathered} \tag{9}$$

Solving the second order variational inequality we find the function χ satisfying the following inequality

$$U \leq \chi V \tag{10}$$

where

$$\chi(t) = \max_{m=1,2,\ldots} \{\chi_m(t)\} \tag{11}$$

and $\chi_m\boldsymbol{(t)}$ is a time-dependent function equal to the maximum solution of the following equation

$$Det \begin{vmatrix} a_{11} & a_{12} & 0 & 0 \\ a_{12} & a_{22} + c\chi_m & 0 & -c\chi_m \\ 0 & 0 & a_{11} & a_{12} \\ 0 & -c\chi_m & a_{12} & a_{22} + (c+d)\chi_m \end{vmatrix} = 0 \tag{12}$$

where

$$a_{11} = \chi_m, \qquad a_{12} = \beta(\chi_m - \beta) + \tfrac{1}{2}\tilde{N}(t)\left(\tfrac{m\pi}{l}\right)^2,$$

$$a_{22} = 2\beta^2(\chi_m - \beta) + \left(\tfrac{m\pi}{l}\right)^2 \chi_m \left(e\left(\tfrac{m\pi}{l}\right)^2 - N_o\right) + \tfrac{1}{2}\beta\tilde{N}(t)\left(\tfrac{m\pi}{l}\right)^2 + c\,\chi_m. \tag{13}$$

Using inequality (10) in equation (8) leads to the following inequality

$$\frac{dV}{dt} \leq -2(\beta - \chi)V \tag{14}$$

Solving the first order differential inequality we have the upper bound estimation of functional (5) along arbitrary solution of dynamic equations (1), (2)

$$V(t) \leq V(0)\exp\left[-2\left(\beta - \frac{1}{t}\int_0^t \chi(\tau)\,d\tau\right)t\right] \tag{15}$$

Therefore, if the forces acting in the tubes are stationary and ergodic processes the almost sure stability condition is written in the form

$$\beta \geq E\chi \tag{16}$$

where $\boldsymbol{E}$ is a mathematical expectation.

4. Simplified models

If bending energies of both tubes dominate the energy of van der Waals forces the problem of tubes parametric vibrations decouples and the double beam dynamic equations are written in a simplified form

$$w_{,tt} + 2\beta w_{,t} + ew_{,xxxx} + \left(N_o + \tilde{N}(t)\right)w_{,xx} = 0 \tag{17}$$

$$x \in (0, l)$$

$$u_{,tt} + 2\beta u_{,t} + eu_{,xxxx} + \left(N_o + \tilde{N}(t)\right)u_{,xx} + du = 0 \tag{18}$$

Using the method described in the Section 3 the almost sure stability condition has the following form

$$\beta_1 \geq E \max_{m=1,2,\dots} \left\{ \frac{\left|\beta^2 + \left(\frac{m\pi}{l}\right)^2 \tilde{N}(t)/2\right|}{\sqrt{\beta^2 + \left(\frac{m\pi}{l}\right)^2 \left[e\left(\frac{m\pi}{l}\right)^2 - N_o\right] + d}} \right\} \tag{19}$$

The farther simplification is done if the energy of Winkler foundation can be neglected and the constant d in denominator in equation (19) is omitted.

5. Results

Stability boundaries are calculated for the following data: l=100 nm, e =3.626 10^{-6} m/s^2, $R = 8.5$ nm,c =2.376 10^{35} 1/ms^2, N=0÷2.275 10^{17} m^2/s^2

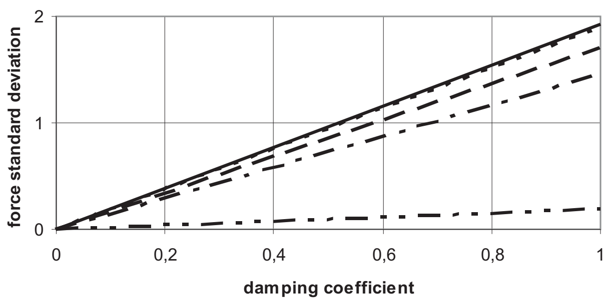

Figure 1 Stability domains for changing constant component of axial force N_o and $d = c$

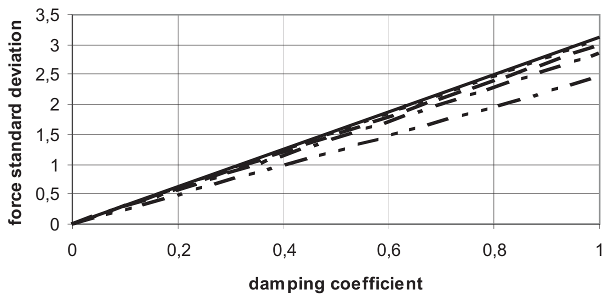

Figure 2 Stability domains calculated according to the simplified approach

Stability regions are situated under straight lines and are determined for changing values of force constant component :$N_o = 0$ - continuous line, $N_o = 10^{16}$ - dotted line, $N_o = 5 \cdot 10^{16}$ - broken line, $N_o = 10^{17}$ - dotted broken line, $N_o = 2.275 \cdot 10^{17}$ - double-dotted broken line. They are calculated using equations (11), (12) and (16). Stability domains calculated according to the simplified approach (19), where van der Waals coupling between tubes is neglected, are shown in Fig. 2. It is seen that the simplified approach is erroneous as differences are large.

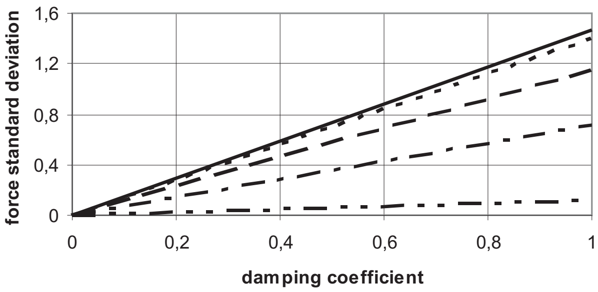

Figure 3 Stability regions for the changing values of force constant component and d=2c

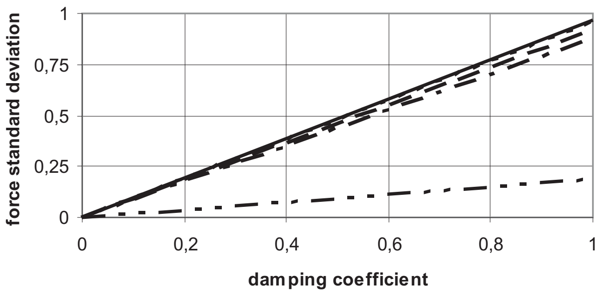

Figure 4 Stability domains for the weaker Winkler foundation d=$c/5$

Stability regions calculated for the more stiff Winkler foundation are shown in Fig. 3 where the double-dotted broken line corresponds to $N_o = 1.31 \cdot 10^{17}$. Stability regions calculated for the weaker Winkler foundation $d = c/5$ are shown in Fig. 4: $N_o = 0$ - continuous line, $N_o = 10^{15}$ - dotted line, $N_o = 5 \cdot 10^{15}$ - broken line, $N_o = 10^{16}$ - dotted broken line, $N_o = 5.5 \cdot 10^{16}$ - double-dotted broken line.

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