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Dynamic Stability of Double-Walled Carbon Nanotubes

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Abstract

This paper investigates the stability of a simply supported DWCNT conveying fluid inside its innermost tube. The van der Waals interaction between the adjacent carbon layers is taken into account. The Euler elastic beam model is employed in order to study the dynamic stability behaviour of the system. The aim is to analyse the influence of the density of the conveyed fluid, the length of the tube and the dimensions of its cross section on the critical flow velocity of the fluid in the pipe under consideration and to draw conclusions about the stability of the system. This problem is approached numerically using the spectral Galerkin method. Results reveal that all above mentioned parameters have a significant effect on the stability of the nanotube.

Keywords: Dynamic stability, fluid-conveying carbon nanotubes, van der Waals interaction, critical velocity

1. Introduction

Carbon nanotubes (CNTs) are formed by crystal lattice of carbon atoms in a periodic hexagonal arrangement and have a cylindrical shell shape. Since 1991, these tubes have been used in nanophysics, nanobiology and nanomechanics in nanofluidic devices, nanocontainers for gas storage and nanopipes conveying fluid. They have perfect hollow cylindrical geometry and superior mechanical strength. The flowing fluid can be water, oil, dynamic flow of methane, ethane and ethylene molecules. These flows inside carbon nanotubes have attractive research topic in recent years.

M.Whitby and N.Quirke (2007) considered the problem of fluid-structure interaction in the case of nanoscale. However, the experiments at the nanoscale are difficult and expensive. That is why the continuum elastic models have been used to study the fluid-structure interaction. The carbon nanotubes are considered with Euler- and Timoshenko-beam models.

Yoon et al. (2006) applied the Euler beam model for investigation of a cantilevered carbon nanotube conveying fluid, with or without being embedded into an elastic medium such as polymer. The same authors in 2005 investigated carbon nanotubes, this time simply supported or clamped at both ends. They obtained the critical flow velocity of the transported fluid in the case of loss of stability of the pipe. The numerical results indicate that the flowing fluid has a substantial effect on vibrational frequencies of the system. On the other hand, their results showed that surrounding elastic medium influence on the effect of internal moving fluid on the vibration of the system.

L. Wang (2009) investigated double-walled carbon nanotubes (DWCNT) with flowing fluid. Y. Yan et al. (2009) studied the instability of triple-walled carbon nanotubes (TWCNT) conveying fluid based on the Euler–Bernoulli beam model. The obtained critical flow velocities of the transported fluid are by a pitchfork bifurcation and a Hamiltonian Hopf bifurcation. The Van der Waals interactions between different carbon nanotubes are taken into account. Numerical results show that these interactions have influence on the natural frequencies and the stability of nanotubes.

E. Ghavanloo et al. (2010) investigated multi-walled carbon nanotubes (MWCNT) as an elastic Euler–Bernoulli beam in order to study the stability of the system. Y. Kuang et al. (2009) considered the influence of the geometric nonlinearity and the nonlinearity of van der Waals forces on the vibration of the double-walled carbon nanotubes conveying fluid. R. Tuzun et al. (1996) investigated nanotubes with flowing fluid. The conclusion of their paper is that the dynamic behaviour of the fluid depends on the physical and geometric characteristics of the pipe and the density of the fluid.

2. Formulation of the problem and method of the solution

A double-walled carbon nanotube (DWCNT) with van der Waals interaction between the adjacent layers is considered herein. A fluid with constant velocity is flowing in the nanotube. The differential equations of the free transverse vibrations of the pipe, shown by Y. Yan et al. (2007), are:

$$EI_1\frac{\partial^4 w_1}{\partial x^4}+m_f V^2\frac{\partial^2 w_1}{\partial x^2}+2m_f V\frac{\partial^2 w_1}{\partial x\partial t}+\left(m_f+m_{p1}\right)\frac{\partial^2 w_1}{\partial t^2}=p_1; \qquad (1)$$

$$EI_2\frac{\partial^4 w_2}{\partial x^4}+m_{p2}V^2\frac{\partial^2 w_2}{\partial t^2}=p_2. \qquad (2)$$

Here x is the axis coordinate, t is the time, w_1 and w_2 are respectively the transverse displacements of the innermost and the outermost layer of DWCNT. E is the modulus of the linear deformations. The names I_1, I_2 and m_{p1}, m_{p2} are respectively the moments of inertia of the cross-section and the masses per unit length of the innermost and outermost layers of the nanotube. m_f is the mass of the flowing fluid per unit length of the pipe. V is the velocity of the flowing fluid. p_1 and p_2 are the van der Waals forces between the two adjacent layers of the pipe. They act respectively on the innermost (p_1) and on the outermost (p_2) layers of the tube.

These interaction forces are expressed by X.He et al. (2005) as follows:

$$p_1=c_{12}\left(w_1-w_2\right); \qquad (3)$$

$$p_2=c_{21}\left(w_2-w_1\right); \qquad (4)$$

$$c_{12} = -R_2\left(\frac{1001\pi\varepsilon\sigma^{12}}{3a^4}E_{12}^{13} - \frac{1120\pi\varepsilon\sigma^6}{9a^4}E_{12}^{7}\right);$$
$$c_{21} = -R_1\left(\frac{1001\pi\varepsilon\sigma^{12}}{3a^4}E_{12}^{13} - \frac{1120\pi\varepsilon\sigma^6}{9a^4}E_{12}^{7}\right); \tag{5}$$

$$E_{12}^{7} = \left(R_1 + R_2\right)^{-7}\int_0^{\pi/2}\frac{d\theta}{\left(1 - k_{12}\cos^2\theta\right)^{3.5}}; \tag{6}$$

$$E_{12}^{13} = \left(R_1 + R_2\right)^{-13}\int_0^{\pi/2}\frac{d\theta}{\left(1 - k_{12}\cos^2\theta\right)^{6.5}}; \tag{7}$$

$$k_{12} = \frac{4R_1R_2}{\left(R_1 + R_2\right)^2}. \tag{8}$$

R_1 and R_2 are the inner radii of the two layers of the nanotube, a is the C–C bond length. ε is the depth of the potential, σ - a parameter that is determined by the equilibrium distance (X.He et al. 2005).

For convenience of the solution of the differential equations (1) and (2) non-dimensional coordinates are introduced:

$$\xi = \frac{x}{L};\ \eta_1 = \frac{w_1}{L};\ \eta_2 = \frac{w_2}{L};\ \tau = \sqrt{\frac{EI_1}{m_f + m_{p1}}}\frac{t}{L^2};\ u = \sqrt{\frac{m_f}{EI_1}}LV;\ \beta_1 = \frac{m_f}{m_f + m_{p1}}; \tag{9}$$

$$\beta_2 = \frac{m_{p2}I_1}{\left(m_f + m_{p1}\right)I_2};\ \bar{c}12 = \frac{c_{12}L^4}{EI_1};\ \bar{c}21 = \frac{c_{21}L^4}{EI_2}.$$

L is the length of the nanotube. Then equations (1) and (2) rewritten in dimensionless form are:

$$\frac{\partial^4\eta_1}{\partial\xi^4} + u^2\frac{\partial^2\eta_1}{\partial\xi^2} + 2\sqrt{\beta_1}u\frac{\partial^2\eta_1}{\partial\xi^2\partial\tau^2} + \frac{\partial^2\eta_1}{\partial\tau^2} - \bar{c}12\left(\eta_1 - \eta_2\right) = 0; \tag{10}$$

$$\frac{\partial^4\eta_2}{\partial\xi^4} + \beta_2\frac{\partial^2\eta_2}{\partial\xi^2} + -\bar{c}21\left(\eta_2 - \eta_1\right) = 0. \tag{11}$$

The spectral Galerkin method is applied to approximate the solution of the boundary value problem (10), (11). According to this method, an approximate solution is sought in the form:

$$\eta_1 = \sum_{i=1}^{n} q_i(\tau)\phi_i(\xi);\ \eta_2 = \sum_{i=1}^{n} q_{i+n}(\tau)\phi_i(\xi). \tag{12}$$

In these expressions, $q_i(\tau)$ and $q_{i+n}(\tau)$ are unknown functions. $\phi_i(\xi)$ are basic functions satisfying the boundary conditions of the tube. The eigenfunctions for the nanotube with stationary fluid $(V=0)$ are used as basic functions in the present paper.

Substituting (12) in equations (10) and (11) one obtains the residual functions, which do not vanish identically since $\eta_1(\xi,\tau)$ and $\eta_2(\xi,\tau)$ are not exact solutions of equations (10) and (11) . Here, and in the sequel, dots denote derivatives with respect to τ and primes denote derivatives with respect to ξ .

$$R_1(\xi,\tau)=\sum_{i=1}^{n}\left[q_i\phi_i^{IV}+u^2q_i\phi_i^{II}+2\sqrt{\beta_1}u\dot{q}_i\phi_i^{I}+\ddot{q}_i\phi_i-\bar{c}_{12}\left(q_n-q_{i+n}\right)\phi_i\right]; \tag{13}$$

$$R_2(\xi,\tau)=\sum_{i=1}^{n}\left[q_{i+n}\phi_i^{IV}+\beta_2\ddot{q}_{i+n}\phi_i-\bar{c}_{12}\left(q_{i+n}-q_i\right)\phi_i\right]. \tag{14}$$

According to the standard Galerkin procedure, the residual functions $R_1(\xi,\tau)$ and $R_2(\xi,\tau)$ should be orthogonal to the basic functions in the area $\xi\in[0;1]$:

$$\int_0^1 R_1(\xi,\tau)\phi_s(\xi)\,d\xi=0,\ s=1,\dots,n \tag{15}$$

$$\int_0^1 R_2(\xi,\tau)\phi_s(\xi)\,d\xi=0,\ s=1,\dots,n \tag{16}$$

The result of the application of (15) and (16) is a system of $2n$ differential equations about the unknown functions $q_i(\tau)$. This system for the differential equations (10) and (11) is:

$$\int_0^1\sum_{i=1}^{n}\phi_s\left[q_i\phi_i^{IV}+u^2q_i\phi_i^{II}+2\sqrt{\beta_1}u\dot{q}_i\phi_i^{I}+\ddot{q}_i\phi_i-\bar{c}_{12}\left(q_n-q_{i+n}\right)\phi_i\right]d\xi=0; \tag{17}$$

$$\int_0^1\sum_{i=1}^{n}\phi_s\left[q_{i+n}\phi_i^{IV}+\beta_2\ddot{q}_{i+n}\phi_i-\bar{c}_{12}\left(q_{i+n}-q_i\right)\phi_i\right]d\xi=0. \tag{18}$$

For a pipe with a static scheme of a simply supported beam the basic functions are:

$$\phi_i(\xi)=\sin\left(\lambda_i\xi\right). \tag{19}$$

The following expressions are valid:

$$\delta_{si}=\int_0^1\phi_s\phi_i\,d\xi=\begin{cases}0.5, & s=i\\ 0, & s\neq i\end{cases}; \tag{20}$$

$$b_{si} = \int_0^1 \phi_s \phi_i^I \, d\xi = \begin{cases} \dfrac{\lambda_s \lambda_i \left[1-\left(-1\right)^{s+i}\right]}{\lambda_s^2 \lambda_i^2}, \; s \neq i \\ 0, \; s = i \end{cases}; \tag{21}$$

$$d_{si} = \int_0^1 \phi_s \phi_i^{II} \, d\xi = -0.5\lambda_i^2 \delta_{si}. \tag{22}$$

The expressions (20), (21) and (22) are substituted in (17) and (18). Then the following system of $2n$ pcs second-order differential equations for the unknown functions $q_i\left(\tau\right)$ is obtained:

$$\sum_{i=1}^{n} \left[\delta_{si}\lambda_i^4 q_i + u^2 \delta_{si} q_i + 2\sqrt{\beta_1} u \delta_{si} \dot{q}_i + \delta_{si} \ddot{q}_i - \bar{c}12\left(q_n - q_{i+n}\right)\delta_{si} \right] = 0; \tag{23}$$

$$\sum_{i=1}^{n} \left[\lambda_i^4 \delta_{si} q_{i+n} + \beta_2 \delta_{si} \ddot{q}_{i+n} - \bar{c}21\left(q_{i+n} - q_i\right)\delta_{si} \right] = 0. \tag{24}$$

The system of differential equations (23) and (24) can be written in the following matrix form:

$$\left|M\right| \ddot{q} + \left|C\right| \dot{q} + \left|K\right| q = 0. \tag{25}$$

The characteristic equation of the system (25) is:

$$\det\left(X\right) = 0. \tag{26}$$

The members of the matrix X are obtained by the following formula:

$$X_{km} = \lambda^2 M_{km} + \lambda C_{km} + K_{km}. \tag{27}$$

It is well known that the knowledge of the roots λ of the characteristic equation λ (25) is sufficient for the stability analysis. The system is stable if the real parts of the roots are negative. The characteristics of the system and the velocity of the transported fluid influence on these roots. Then the critical velocity of the flowing fluid V_{cr} can be obtained.

3. Numerical results

A double-walled carbon nanotube (DWCNT) supported as a simple beam is considered. The thickness of the two adjacent layers of the tube and the gap between them are $0.34\ nm$ (Fig. 1). The parameters that are used to calculate van der Waals's forces according to formula (5) are: $\varepsilon = 2.968\ meV$, $a = 1.42\ \overset{o}{\mathrm{A}}$ and $\sigma = 3.407\ \overset{o}{\mathrm{A}}$. The characteristics of the material of the tube are: modulus of linear elasticity $E = 1\ TPa$, density $2.3\ g/cm^3$. Several types of flowing fluid are investigated with its density ranging in the interval $0.5-1.5\ g/cm^3$.

The results obtained show the relationship between the density of the fluid and its critical velocity for tubes with lengths $L = 10\ \mu m,\ 20\ \mu m$ and $30\ \mu m$ and for two different cross-sections of the pipe (Fig. 2 and 3). The first cross-section under consideration is with a radius $R_1 = 12\ nm$ (inner radius of the first layer) and $R_2 = 12.64\ nm$ (inner radius of the second layer). The second cross-section is with $R_1 = 20\ nm$ and $R_2 = 20.64\ nm$.

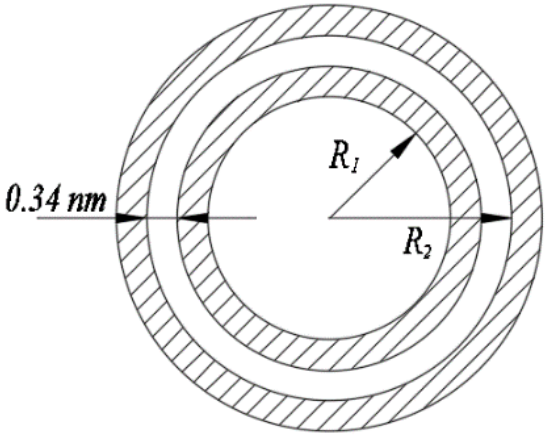

Fig.1. Cross-section of the tube

The results are shown in Fig.2 and Fig.3.

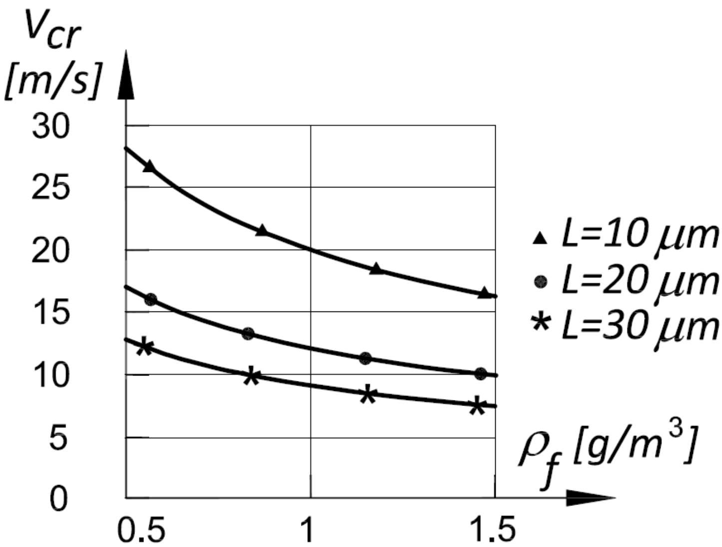

Fig.2. DWCNT with $R_1 = 12\ nm$ and $R_2 = 12.64\ nm$

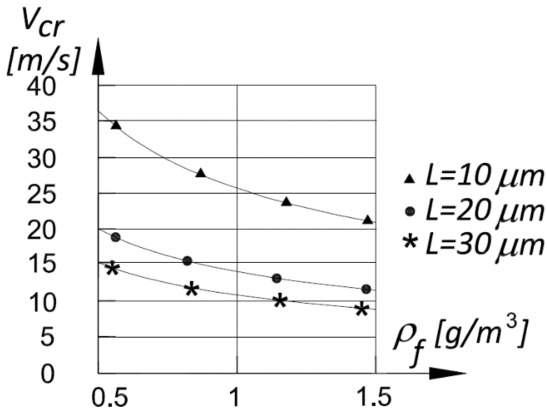

Fig.3. DWCNT with $R_1 = 20$ *nm* and $R_2 = 20.64$ *nm*

4. Conclusions

The results from numerical investigations show that for all considered tubes the critical velocity of the flowing fluid is reduced when the density of the fluid is increasing. The pipes with bigger length are less stable. Amongst the pipes with different cross section, more stable is the one with the largest radii R_1 and R_2. All obtained critical velocities in this paper correspond to loss of stability of the tube in divergent form.

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