FREE VIBRATION OF THE WATER-FILLED DOUBLE-WALLED CARBON NANOTUBES BASED ON A THREE SHELL-POTENTIAL FLOW MODEL

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Summary A three shell-potential flow model is developed to study the free vibration of double-walled carbon nanotubes (DWCNTs) conveying water. The inner and outer walls of DWCNTs are coupled via the van der Waals (vdW) interaction, meanwhile, vdW forces between the inner tube and water are also considered. Results reveal that the internal moving fluid plays an important role in the instability of system. The critical flow velocities—associated with twice divergence and flutter—are also determined.

INTRODUCTION

The research topic on the system of water stored or conveyed inside the carbon nanotubes (CNTs) has become an attractive object in recent years. Up till now, considerable effort has been made to explore the dynamical behavior of water-filled CNTs, nevertheless, there is little systematic consideration concerning the density of water in CNT in these literature, and the overall density is unnaturally fixed to $1g/cm^3$. Water molecules, in fact, show at least two different ways of filling CNT called "single-file mode" and "layered mode" [1]. Fortunately, some researchers have realized the problem and put considerable attention on it.

Motivated by these earlier studies, for the first time, we develop a three shell-potential flow model for the water-filled DWCNTs. The model greatly reduces the time required to simulate the effect of absorbed fluid on the vibration mode of CNTs. The study can also offer a theoretical explanation for the experimental observation and molecular dynamics simulations available in particular cases. As will be shown below, based on the model, discusses in detail are performed.

THREE SHELL-POTENTIAL FLOW MODEL

The DWCNT-water system comprises three constituent parts, i.e., the DWCNTs, the absorbed layer of water molecules and the water flow in the center of the inner tube. The DWCNTs and the internally absorbed layer of water are modelled as three-layer thin shells coupled via the interlayer vdW interaction, and the water in the center of the inner tube is considered as the potential flow. By using the shell theory, the governing equations of motion are stated as

$$D\nabla^4 w_1+\rho_t h\frac{\partial^2 w_1}{\partial t^2}=c_1\left(w_2-w_1\right)-c_2\left(w_1-w_3\right)+\frac{1}{R_1}\frac{\partial^2 F_1}{\partial x^2} \tag{1}$$

$$D\nabla^4 w_2+\rho_t h\frac{\partial^2 w_2}{\partial t^2}=-\frac{c_1 R_1}{R_2}\left(w_2-w_1\right)+\frac{1}{R_2}\frac{\partial^2 F_2}{\partial x^2} \tag{2}$$

$$\gamma\frac{\partial^2 w_3}{\partial x^2}+\frac{R_1}{R_3}c_2\left(w_1-w_3\right)-p=\rho_f\frac{\partial^2 w_3}{\partial t^2} \tag{3}$$

$$\nabla^4 F_i=-\frac{Eh}{R_i}\frac{\partial^2 w_i}{\partial x^2} \tag{4}$$

$$p=\rho_{water}\frac{L}{m\pi}\frac{I_n\left(m\pi R_f/L\right)}{I_n'\left(m\pi R_f/L\right)}\left(\frac{\partial}{\partial t}+U\frac{\partial}{\partial x}\right)^2 w_3 \tag{5}$$

where x and θ are the axial and circumferential (angular) coordinates, respectively, t the time, F_i the stress function; $\nabla^4=\left[\frac{\partial^2}{\partial x^2}+\frac{1}{R_i^2}\frac{\partial^2}{\partial\theta^2}\right]^2$ a differential operator, I_n the modified Bessel function of order n, prime($'$) the derivative with respect to the spatial variable. For DWCNTs ($i=1$ for the inner tube and $i=2$ for the outer tube). R_i the radius, w_i the radial displacement, E Young's modulus, h the tube thickness, D the flexural rigidity, ρ_t the mass density per unit bulk, L the length; For water shell, ρ_f the mass density per unit area, R_3 the radius, w_3 the radial displacement, γ the CNT–water surface tension, ρ_{water} the mass density per unit bulk of the potential flow, p the radial pressure executed on the water shell due to the water in the center of the DWCNTs, c_1 and c_2 corresponding to the vdW interaction coefficient between the inner and outer tubers and that of the inner tube and water shell, respectively.

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For simply supported water-filled DWCNTs, the solution of Eqs. (1-3) can be obtained by

$$w_1 = \sum_{m=1}^{2} A_{m,n}(t)\sin(m\pi x/L)\cos(n\theta), \tag{6}$$

$$w_2 = \sum_{m=1}^{2} A_{m+2,n}(t)\sin(m\pi x/L)\cos(n\theta), \tag{7}$$

$$w_3 = \sum_{m=1}^{2} A_{m+4,n}(t)\sin(m\pi x/L)\cos(n\theta), \tag{8}$$

where $A_{m,n}(t)$ is the unknown function of time. m, n denote the axial and circumferential wave numbers, respectively. Using the same method as Ref. [2], we can get a matrix form, where [C] is the coefficient matrix, then the characteristic equation of the coupled system is stated as

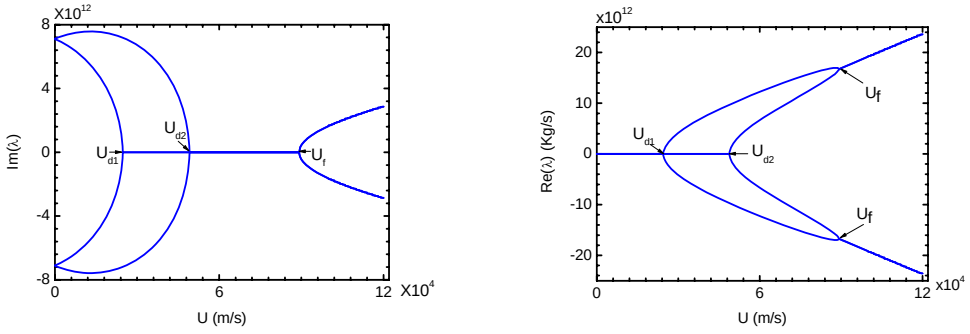
$$\det(\lambda[I]-[C]) = 0, \tag{9}$$

where [I] is an identity matrix, λ is the eigenvalue of the system. Generally, the eigenvalue is a complex number. Obviously, the eigenvalue is a function of the flow velocity.

RESULTS AND DISCUSSIONS

The dynamical simulations are performed on a DWCNT at 300 K. The values used in the paper are $\rho_t = 2.27$ g/cm^3, $h = 0.1nm$, $Eh = 360$J/m^2, $D = 2eV$, $R_1 = 1.356nm$, $n = 5$, $L/R_1 = 10$, and the initial separation between the two walls is 0.34 nm. The values of ρ_f, γ, c_1, c_2 and s can be extracted by fitting the double shell model to the MD simulations [3, 4].

The diagrams for the evolution of the real parts (which represent the frequencies of water shell) and imaginary parts (which is regarded as a ‘‘damping mechanism’’) of the eigenvalues of the system as the flow velocity U are plotted in Fig. 1. It is clear from Fig. 1(a) that, the imaginary parts of the eigenvalues decrease as the flow velocity increases; when the flow velocity is up to U_{d1}, a pitchfork bifurcation appears, and then the tube loses stability due to having a positive real part, as shown in Fig. 1(b). This indicates that the tube absorbs energy from the flow to amplify vibration. As the flow velocity is continually up to U_{d2}, obviously, the second pitchfork bifurcation presents; Thereafter, the third instability (hopf bifurcation) comes at U_f, After $U > U_f$, the system becomes unstable once more.



(a) Imaginary part (b) Real part

Fig. 1. Evolution of the imaginary and real parts of the eigenvalue with velocity

CONCLUSIONS

Water-filled DWCNTs are modeled by three shell-potential flow theory with consideration of the vdW interactions. The numerical simulations reveal that as the flow velocity increases, the system has a destabilizing way to get through multibifurcations of the first and second pitchforks and Hopf bifurcations in turn.

References

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