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Elastic vibrations of a cylindrical nanotube with the effect of surface stress and surface inertia

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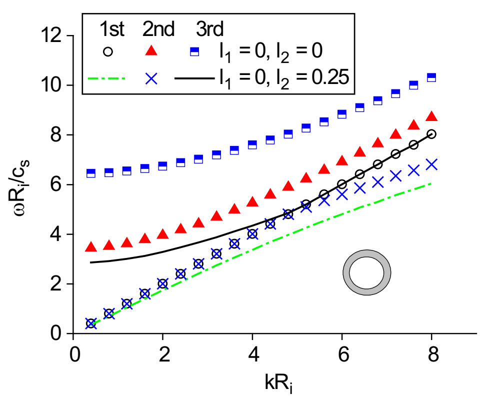
HIGHLIGHTS

- Surface stress and surface inertia have been taken into account to study the acoustic vibration of a nanotube.
- Both surface stress and surface inertia have significant influence on the vibration behavior of the nanotube.
- Due to the surface effect, resonant frequency of some vibration modes may be the same as that of lower order by the classical elasticity.
- The surface effect may either decrease or increase the Raman shift compared to the classical results.

GRAPHICAL ABSTRACT

The dispersion relation of torsion mode demonstrated that the effect of surface inertia may render the vibration frequency of the third order consistent with the lowest one in conventional elasticity.



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ABSTRACT

Vibration frequency analysis of nanostructures may be essential for study of their thermal conductivity and mechanical characterization. Given the high surface-to-volume ratio, the elastic vibrations of an infinitely long cylindrical nanotube have been studied by considering both the effects of surface stress and that of surface inertia within the framework of surface elasticity. The phonon dispersion and the resonant frequencies for the specific vibration modes have been calculated. Numerical results have indicated that the surface stress and the surface inertia have equally important effect on the vibration behavior of the nanotube that may depend on the vibration modes as well. Due to the surface effect, the vibration modes of lower order by the classical elasticity may be indeed the modes of higher order. The surface effect on the low-frequency Raman shift has also been found.

1. Introduction

Due to the development of synthesis technology, nanotubes of a wide variety of materials have been synthesized. As nanotubes exhibit prominent properties, they can be used as fundamental components of functional assemblies and systems which may play an important role in the future nanotechnology [1–4]. Among many of the potential applications, phonon behaviors can be involved since phonon spectrum plays a key part in the temperature-dependent transport [5,6], superconductivity [7,8], and optical characterization [9–11] of nanotubes. Consequently researchers have devoted abundant efforts to study their elastic

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vibrational properties [12–17]. In those works, nanotubes were considered as cylindrical shells, and the vibrations were dealt with classical isotropic or anisotropic continuum elasticity models.

It is noteworthy however that many nanostructures exhibit size dependent elastic behavior when characterized by the conventional elasticity. To capture such effect on the vibration behavior, non-classical elasticity like nonlocal elasticity has been adopted in some investigations [18–20]. Owing to the high ratio of surface area to volume in nanostructures, the size dependent behavior may be attributed to the surface effect as shown by the experiment of Chen et al. [21]. Consequently, many efforts [22–25] have recently been made to study the surface effect on the mechanical behavior of nanostructure by surface elasticity which was firstly proposed by Gurtin and Murdoch [26]. According to the theory, the surface can actually be treated as an elastic membrane without thickness perfectly bonded to the bulk. In the limited studies on the dynamic behavior of nanostructures by surface elasticity, the mass density of the surface has been neglected and hence the surface effect, which indeed is the effect of surface stress, has been demonstrated to be significant. But according to the thermodynamic definitions of the surface properties [27], the surface may also possess mass which actually appears in the original surface elasticity model proposed by Murdoch [28], the surface inertia effect should be captured as well when studying the vibration of nanostructures. In this regard, one of the present authors [29] has preliminary shown for nanowires, the effect of surface inertia can be significant.

Given the higher ratio of surface area to volume in nanotubes than in nanowires, the surface effect on the vibrations is anticipated to be prominent. Therefore, in this paper, we are motivated to study the elastic vibrations of nanotubes by accounting for both the surface stress and surface inertia.

2. Problem formulation

Let us consider an infinitely long cylindrical nanotube, whose outer radius and inner radius are respectively R_o and R_i. To consider the surface effect, we take advantage of the surface elasticity proposed by Gurtin and Murdoch [26]. According to the theory, there is a linear relationship between surface stress and surface strain, that is

$$\sigma^s_{\alpha\beta} = \lambda^s \varepsilon_{\gamma\gamma}\delta_{\alpha\beta} + 2\mu^s \varepsilon_{\alpha\beta} \tag{1}$$

where $\varepsilon_{\alpha\beta}$ is the tensor of surface strain, $\delta_{\alpha\beta}$ is the Kronecker delta, λ^s and μ^s are the surface Lame constants. In Eq. (1), the residual surface stress has been neglected. To capture the effect of surface inertia, we assume the mass density of the surface is ρ_s which has a dimension of $\mathrm{kg/m^2}$.

With the presence of surface effect, the Euler–Lagrange equations for vibrations can be obtained easily if the Lagrangian of a nanotube is expressed explicitly. Herein, we only give the final results. The motion equations in the bulk can be obtained as

$$\nabla\cdot\boldsymbol{\sigma} = \rho\frac{\partial^2 \mathbf{u}}{\partial t^2} \tag{2}$$

Due to the assumption of traction-free boundary conditions on both inner and outer free surfaces, the motion equations at the outer surface $r = R_o$ read [30]

$$-R_o\sigma_{rr} - \sigma^s_{\theta\theta} = \rho_s R_o \frac{\partial^2 u_r}{\partial t^2}, \tag{3}$$

$$-R_o\sigma_{r\theta} + \frac{\partial \sigma^s_{\theta\theta}}{\partial\theta} + R_o\frac{\partial\sigma^s_{\theta z}}{\partial z} = \rho_s R_o\frac{\partial^2 u_\theta}{\partial t^2}, \tag{4}$$

$$-R_o\sigma_{rz} + \frac{\partial \sigma^s_{\theta z}}{\partial\theta} + R_o\frac{\partial\sigma^s_{zz}}{\partial z} = \rho_s R_o\frac{\partial^2 u_z}{\partial t^2}. \tag{5}$$

and at the inner surface $r = R_i$

$$R_i\sigma_{rr} - \sigma^s_{\theta\theta} = \rho_s R_i \frac{\partial^2 u_r}{\partial t^2}, \tag{6}$$

$$R_i\sigma_{r\theta} + \frac{\partial \sigma^s_{\theta\theta}}{\partial\theta} + R_i\frac{\partial\sigma^s_{\theta z}}{\partial z} = \rho_s R_i\frac{\partial^2 u_\theta}{\partial t^2}, \tag{7}$$

$$R_i\sigma_{rz} + \frac{\partial \sigma^s_{\theta z}}{\partial\theta} + R_i\frac{\partial\sigma^s_{zz}}{\partial z} = \rho_s R_i\frac{\partial^2 u_z}{\partial t^2}. \tag{8}$$

As displayed in Eqs. (3)–(8), the surface effect makes the boundary equations different from those of classic elasticity.

The bulk motion Eq. (2) can be expressed in the form of standard wave equations. To that end, we set the displacement fields as

$$\mathbf{u} = \nabla\varphi + \nabla\times(\psi\mathbf{e}_z) + \nabla\times(\nabla\times\chi\mathbf{e}_z) \tag{9}$$

where φ, ψ and χ are potential functions, and $\mathbf{e}_z$ is the unit vector along the axis of the cylinder. Combining Eq. (9) with the geometric relation

$$\begin{aligned} &\varepsilon_r = \frac{\partial u_r}{\partial r}; && \varepsilon_{r\theta} = \frac{1}{2}\left(\frac{1}{r}\frac{\partial u_r}{\partial\theta} + \frac{\partial u_\theta}{\partial r} - \frac{u_\theta}{r}\right); \\ &\varepsilon_\theta = \frac{1}{r}\frac{\partial u_\theta}{\partial\theta} + \frac{u_r}{r}; && \varepsilon_{\theta z} = \frac{1}{2}\left(\frac{1}{r}\frac{\partial u_z}{\partial\theta} + \frac{\partial u_\theta}{\partial z}\right); \\ &\varepsilon_z = \frac{\partial u_z}{\partial z}; && \varepsilon_{zr} = \frac{1}{2}\left(\frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z}\right). \end{aligned} \tag{10}$$

and Hook's law

$$\sigma_{ij} = \lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}, \tag{11}$$

we then find that the motion equations in the bulk can be described in the following simple form:

$$\nabla^2\varphi = \frac{1}{c_d^2}\frac{\partial^2\varphi}{\partial t^2}, \tag{12}$$

$$\nabla^2\psi = \frac{1}{c_s^2}\frac{\partial^2\psi}{\partial t^2}, \tag{13}$$

$$\nabla^2\chi = \frac{1}{c_s^2}\frac{\partial^2\chi}{\partial t^2}, \tag{14}$$

where $c_d^2 = (\lambda + 2\mu)/\rho$, $c_s^2 = \mu/\rho$ with ρ the density, μ and λ are the Lame constants in the bulk.

The solutions with circular frequency ω satisfying the Eqs. (12)–(14) can be expressed as

$$\varphi = \sum_n [A_{1n}F_{1n}(\alpha r) + B_{1n}G_{1n}(\alpha r)]e^{i(n\theta + kz - \omega t)} \tag{15}$$

$$\psi = \sum_n [A_{2n}F_{2n}(\beta r) + B_{2n}G_{2n}(\beta r)]e^{i(n\theta + kz - \omega t)} \tag{16}$$

$$\chi = \sum_n [A_{3n}F_{2n}(\beta r) + B_{3n}G_{2n}(\beta r)]e^{i(n\theta + kz - \omega t)} \tag{17}$$

where $\alpha = |\omega^2/c_d^2 - k^2|^{1/2}$, $\beta = |\omega^2/c_s^2 - k^2|^{1/2}$ with k the wavenumber, A_{1n}, A_{2n}, A_{3n}, B_{1n}, B_{2n} and B_{3n} are constants to be determined, and

$$F_{1n}(\alpha r) = J_n(\alpha r)H(\omega^2/c_d^2 - k^2) + I_n(\alpha r)H(k^2 - \omega^2/c_d^2), \tag{18}$$

$$F_{2n}(\beta r) = J_n(\beta r)H(\omega^2/c_s^2 - k^2) + I_n(\beta r)H(k^2 - \omega^2/c_s^2), \tag{19}$$

$$G_{1n}(\alpha r) = Y_n(\alpha r)H(\omega^2/c_d^2 - k^2) + K_n(\alpha r)H(k^2 - \omega^2/c_d^2), \tag{20}$$

$$G_{2n}(\beta r) = Y_n(\beta r)H(\omega^2/c_s^2 - k^2) + K_n(\beta r)H(k^2 - \omega^2/c_s^2), \tag{21}$$

with $H()$ the Heaviside jump function, J_n and Y_n the first and second kind Bessel functions of nth order, and I_n and K_n the first and second kind modified Bessel functions of nth order.