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Proc. R. Soc. A 2011 **467**, 860-868 first published online 30 June 2010
doi: 10.1098/rspa.2010.0265

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Published online 30 June 2010

Dynamic modelling of a single-walled carbon nanotube for nanoparticle delivery

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In this paper, the dynamic behaviour of a single-walled carbon nanotube (SWCNT) for nanoparticle delivery is studied using non-local elasticity theory. The response of the delivery system depends on the time history and velocity of the moving nanoparticle. In addition, the interaction between the SWCNT and the moving nanoparticle, and the foundation of the SWCNT can also influence the dynamic behaviour of the system. The effects of foundation stiffness, confined stiffness, velocity ratio, non-local parameter and travel time on the behaviour are analysed using the Runge–Kutta method. The numerical solution is in agreement with the analytical result for the special case. The numerical analysis shows that increasing the non-local parameter, confined stiffness and foundation stiffness decreases the dynamic displacement of SWCNT. However, increasing the velocity ratio increases the maximum displacement.

Keywords: single-walled carbon nanotube; nanoparticle delivery; non-local elasticity theory

1. Introduction

Carbon nanotubes (CNTs) have many potential applications in nanobiological devices and nanomechanical systems such as fluid conveyance and nanoparticle delivery because of excellent mechanical properties, chemical and thermal stability and hollow geometry (Dirote 2004; O'Connell 2006; Yudasaka *et al.* 2008; Ottenhouse 2009). The space inside the CNT can be considered as the nanocontainer and the fullerenes, e.g. C_{60}, C_{70}, C_{78}, C_{80} and C_{84}, can be considered as the nanoparticle. This concept can be extended to study the delivery of a drug. CNTs have gained significant attention as targeted drug delivery nanocapsules in recent years. For example, Hilder & Hill (2007) used a hybrid discrete–continuum formulation to describe the interaction of the drug molecule cisplatin with a CNT. Chen *et al.* (2009) performed a molecular dynamics simulation to investigate the dynamic properties and energetics of the protein/peptide drug during its transport through CNTs. They found that the van der Waals interactions can be influenced by varying the lengths and diameters of the CNT. Bhirde *et al.* (2009) used CNT-based drug delivery for cancer therapy and demonstrated that targeted CNT drug delivery resulted in a rapid decrease in tumour size in mice compared with a non-targeted CNT control.

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Received 22 May 2010
Accepted 2 June 2010

In addition, some researchers have studied the mechanical behaviour of nanoparticles encapsulated into a CNT (Qian *et al.* 2001; Otani *et al.* 2003; Baowan *et al.* 2007; Cox *et al.* 2007; Warner *et al.* 2009). For example, Qian *et al.* (2001) used a combined continuum/molecular dynamics approach to analyse the interaction between C_{60} and different armchair nanotubes. Cox *et al.* (2007) investigated the suction force experienced by either an atom or a C_{60} fullerene molecule located in the vicinity of the open end of a single-walled CNT (SWCNT) and obtained the van der Waals interaction force between the atom or C_{60} fullerene and the SWCNT. Warner *et al.* (2009) studied peapods containing metallofullerenes that were transformed into a CNT and found that they exhibited a confined motion along the axis of the nanotube. Recently, Kiani & Mehri (2010) carried out a dynamic analysis of nanotube structures under the excitation of a moving nanoparticle using the non-local continuum theory. They studied the effects of the scale effect parameter, the slenderness ratio and the moving velocity of the nanoparticle on the dynamic deflection of the nanotube. However, the van der Waals force between the moving nanoparticle and nanotube was ignored. In addition, the effect of the elastic foundation on the deflection was not taken into account in the analysis.

In this paper, we analyse the dynamic displacement in a SWCNT conveying a C_{60} fullerene molecule using the non-local elasticity theory. The theory of non-local elasticity proposed by Eringen (1983) was derived based on solid mechanics. This theory, with a non-local constant, is used to modify the classical elasticity theory and is limited to being applied to a device on the nanometre scale. In recent years, many researchers have applied the non-local elasticity theory to the bending, buckling and mechanical analyses of nanostructures (Lu *et al.* 2006; Wang & Varadan 2007; Wang *et al.* 2007; Lee & Chang 2008). In addition, the theory can be extended to study the vibration frequency of a fluid-conveying CNT (Lee & Chang 2009*a*,*b*). Here, the effects of foundation stiffness, confined stiffness, velocity ratio and travel time on the dynamic displacement of a SWCNT conveying a nanoparticle are investigated based on the non-local elasticity theory.

2. Analysis

According to the non-local elasticity theory, the one-dimensional non-local constitutive relation is given by (Eringen 1983)

$$\sigma(x) - (e_0 a)^2 \frac{\partial^2 \sigma(x)}{\partial x^2} = E\varepsilon(x), \tag{2.1}$$

where σ and ε are the axial stress and strain in the x-direction, E is the Young modulus and $e_0 a$ is the non-local constant. The strains ε can be expressed as

$$\varepsilon = -y \frac{\partial^2 y}{\partial x^2}, \tag{2.2}$$

where y is the transverse displacement.

Based on the definition of the bending moment M, we have

$$M = \int y\sigma(x)\mathrm{d}A. \tag{2.3}$$

Using equations (2.2) and (2.3), the non-local constitutive given by equation (2.1) can be expressed as

$$M - (e_0 a)^2 \frac{\partial^2 M}{\partial x^2} = -EI \frac{\partial^2 y}{\partial x^2}, \tag{2.4}$$

where I is the moment of inertia of the nanotube.

In addition, based on the Bernoulli–Euler beam theory, the equation of transverse vibrations for a SWCNT is expressed by

$$\frac{\partial Q}{\partial x} + F = m_c \frac{\partial^2 y}{\partial t^2} \tag{2.5}$$

and

$$Q - \frac{\partial M}{\partial x} = 0, \tag{2.6}$$

where Q is the shear force, m_c is the mass per unit length for the SWCNT and F is the force acting on the SWCNT, which can be expressed by

$$F = (mg - Wy)\delta(x - vt) - Ky, \tag{2.7}$$

where m is the mass of the moving nanoparticle and the mass moves with a uniform speed v along the centreline in the axial direction, K is an elastic medium constant for the Winkler model that represents the embedding medium, W is a linear spring constant, which is used to simulate the van der Waals force between the moving nanoparticle and the SWCNT, and δ is the Dirac delta function.

Using equations (2.4)–(2.7), the governing equation of dynamic motion for a nanoparticle moving in the nanotube using the non-local elasticity theory can be expressed as

$$\begin{aligned} EI \frac{\partial^4 y}{\partial x^4} + \left[1 - (e_0 a)^2 \frac{\partial^2}{\partial x^2}\right] \left(m_c \frac{\partial^2 y}{\partial t^2} + Ky \right) \\ = \left[1 - (e_0 a)^2 \frac{\partial^2}{\partial x^2}\right] (mg - Wy)\delta(x - vt). \end{aligned} \tag{2.8}$$

In this analysis, a SWCNT is assumed to be embedded in an elastic medium with two simple support ends, as shown in figure 1. The SWCNT, carrying a moving nanoparticle with a constant speed v and having an equivalent bending rigidity EI, is described as a hollow cylindrical tube with length L, inner diameter d and thickness t_c. The corresponding boundary conditions are

$$y(0, t) = y(L, t) = \frac{\partial^2 y(0, t)}{\partial x^2} = \frac{\partial^2 y(L, t)}{\partial x^2} = 0. \tag{2.9}$$

The boundary conditions given by equation (2.9) correspond to zero displacement and zero moment at $x = 0$ and L, respectively.

In addition, the initial conditions for the transverse displacement and velocity of the SWCNT are assumed to be zero. They can be expressed as

$$y(x, 0) = \frac{\partial y(x, 0)}{\partial t} = 0. \tag{2.10}$$

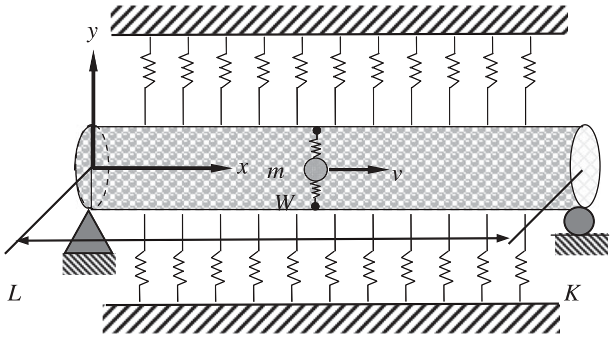

Figure 1. A nanoparticle-carrying SWCNT is assumed to be embedded in an elastic medium with two simple support ends and is described as a hollow cylindrical tube with length L.

Then, the solution of equation (2.8) can be expressed as

$$y(x,t)=\sum_{n=1}^{\infty} y_n(t)\sin\left(\frac{\lambda_n x}{L}\right),\quad \lambda_n=n\pi,\ n=1,2,3,\ldots, \tag{2.11}$$

where $y_n(t)$ is an unknown function of time and $\sin(\lambda_n x/L)$ is the deflection curve for the nth mode of a vibrating simply supported SWCNT.

By substituting equation (2.11) into equation (2.8) and multiplying by $\sin(\lambda_n x/L)$ and then integrating from 0 to L, we can obtain a set of coupled ordinary differential equations as follows:

$$\frac{\mathrm{d}^2 y_n}{\mathrm{d}t^2}+\omega_n^2\left(\frac{1}{(1+\rho^2\lambda_n^2)}+\frac{k}{\lambda_n^4}\right)y_n+\frac{2w}{\lambda_n^4}\omega_n^2\sin\left(\frac{\lambda_n t}{\tau}\right)\sum_{i=1}^{\infty}\sin\left(\frac{\lambda_i t}{\tau}\right)y_i$$
$$=\frac{96\,Y_s\omega_n^2}{(1+\rho^2\lambda_n^2)\lambda_n^4}\sin\left(\frac{\lambda_n t}{\tau}\right), \tag{2.12}$$

where

$$\rho=\frac{e_0 a}{L},\quad w=\frac{WL^3}{EI},\quad k=\frac{KL^4}{EI},\quad \omega_n^2=\frac{\lambda_n^4 EI}{m_c L^4},\quad Y_s=\frac{mgL^3}{48EI}\quad \text{and}\quad \tau=\frac{L}{v}. \tag{2.13}$$

The above parameters ρ, w and k denote the dimensionless non-local parameter, confined stiffness and foundation stiffness, respectively. The non-local parameter is used to reveal the small size effect when dealing with nanostructures. The confined stiffness is relevant to the van der Waals interaction force between the SWCNT and the moving nanoparticle. The stiffness is a parameter that confines a nanoparticle moving along the centreline of the SWCNT. The foundation stiffness is used to represent the local elastic supports of the SWCNT. ω_n is the circular frequency of the SWCNT, Y_s is the static transverse displacement at the mid-span of the SWCNT owing to the nanoparticle weight and τ is the travel time of the moving nanoparticle through the SWCNT.

It is convenient to introduce the following dimensionless parameters:

$$v_{\mathrm{cr}} = \pi\sqrt{\frac{EI}{m_c L^2}} \quad \text{and} \quad \alpha = \frac{v}{v_{\mathrm{cr}}}, \tag{2.14}$$

where v_{cr} denotes the critical speed of the SWCNT carrying a moving nanoparticle, which is defined as the speed at which the moving nanoparticle will excite the SWCNT at its fundamental resonance frequency, and α is the speed ratio.

Equation (2.12) with its initial conditions can be solved by using the fourth-order Runge–Kutta method (Burden & Faires 1985). While neglecting the van der Waals term W (i.e. $W = 0$) in this equation, the solution can be analytically obtained as follows:

$$y(x, t) = \sum_{n=1}^{\infty} \frac{96\beta Y_s}{n^2\pi^4(\eta_n^2 n^2 - \alpha^2)}\left[\sin\left(n\pi\frac{t}{\tau}\right) - \frac{\alpha}{\eta_n n}\sin\left(\eta_n\frac{n^2\pi}{\alpha}\frac{t}{\tau}\right)\right]\sin\left(\frac{n\pi x}{L}\right), \tag{2.15}$$

where

$$\beta = \frac{1}{1 + \rho^2\lambda_n^2} \quad \text{and} \quad \eta_n = \sqrt{\frac{\beta + k}{\lambda_n^4}}. \tag{2.16}$$

3. Results and discussion

This paper studies the effects of foundation stiffness, confined stiffness and travel time on the dynamic behaviour of a SWCNT conveying a nanoparticle using the non-local elasticity theory. The SWCNT is assumed to be a (10,10) nanotube and the geometric and material parameters of the nanotube in the analysis are as follows: $d = 1.36$ nm, $L = 40$ nm, $t_c = 0.35$ nm and $E = 1$ TPa (Cox *et al.* 2007; Lee & Chang 2009*b*,*c*). In order to know the effects of relative parameters on the dynamic displacement of the SWCNT, we assumed that the flow nanoparticle in the SWCNT is C_{60} and its mass is $m = 1.196 \times 10^{-24}$ kg (Cox *et al.* 2007). According to the calculation, the following parameters are obtained: $m_c = 4.32 \times 10^{-15}$ kg/m, $EI = 7.12 \times 10^{-25}$ Nm^2 and $v_{\mathrm{cr}} = 1008$ m s^{-1}.

Figure 2 illustrates the dimensionless displacement of a SWCNT for nanoparticle delivery at $\alpha = 0.1$, $\rho = 0.1$ and $k = 20$ for different dimensionless times and confined stiffnesses. The dimensionless displacement is defined by the displacement at the moving nanoparticle location, y, divided by the static transverse displacement, Y_s, at the mid-span of the SWCNT. The dimensionless time, t/τ, is defined as the ratio of actual time and travel time of the moving nanoparticle through the SWCNT. The value of t/τ is in the range of 0–1. It can be seen that the dimensionless displacement varies with increasing value of t/τ owing to the dynamic effect. The maximum displacement is obtained when the value of t/τ is about 0.5. This is because the moving nanoparticle reaches the mid-span of the SWCNT at $t/\tau = 0.5$. In addition, the confined force between the nanoparticle and the SWCNT is affected owing to different nanoparticle materials. In order to study different nanoparticle delivery behaviours in a SWCNT, different confined stiffnesses of $w = 0$, 50 and 100 were used in the

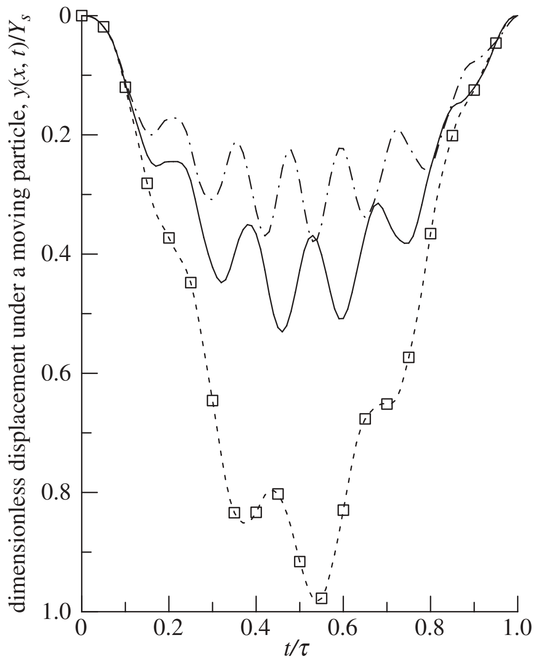

Figure 2. Dimensionless displacement of a SWCNT for nanoparticle delivery at $\alpha = 0.1$, $\rho = 0.1$ and $k = 20$ for different dimensionless times and confined stiffnesses. Open square, $w = 0$ (analytical); dashed line, $w = 0$; solid line, $w = 50$; dashed-dotted line, $w = 100$.

analysis. The value of $w = 0$ implies the confined force is ignored. In the case of $w = 0$, the analytical solution can be obtained, as given in equation (2.15). However, the other cases must be evaluated by using the numerical method. In this paper, the Runge–Kutta method is adopted, and the numerical result is compared with the analytical solution for the case of $w = 0$, as shown in figure 2. It can be seen that the numerical result is in agreement with the analytical solution. It can also be found that increasing the confined stiffness between the nanoparticle and the SWCNT decreases the dynamic displacement of the SWCNT. This is because increasing confined stiffness makes the SWCNT become stiffer.

Figure 3 shows the dimensionless displacement of a SWCNT for nanoparticle delivery at $\alpha = 0.1$, $k = 20$ and $w = 50$ for different dimensionless times and non-local parameters. The displacement decreases with increasing value of the non-local parameter. This is because increasing the non-local parameter leads to an increase in the stiffness of the SWCNT. It is noted that $\rho = 0$ corresponds to a classical solution where the non-local effect is not taken into account in the analysis. Figure 4 depicts the dimensionless displacement of a SWCNT for nanoparticle delivery at $\alpha = 0.1$, $\rho = 0.1$ and $w = 50$ for different dimensionless times and foundation stiffnesses. The dynamic displacement decreases with increasing foundation stiffness. This is because increasing the foundation stiffness leads to an increase in the stiffness of the SWCNT. Figure 5 illustrates the dimensionless displacement of a SWCNT for nanoparticle delivery at $k = 20$, $\rho = 0.1$ and $w = 50$ for different dimensionless times and velocity ratios of the

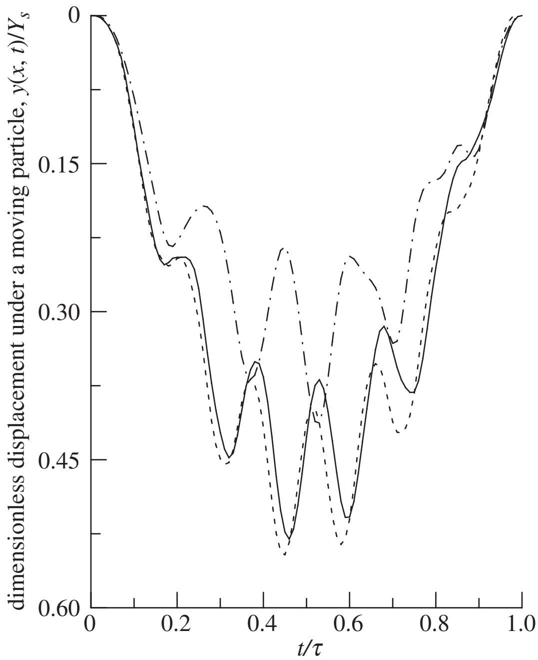

Figure 3. Dimensionless displacement of a SWCNT for nanoparticle delivery at $\alpha = 0.1$, $k = 20$ and $w = 50$ for different dimensionless times and non-local parameters. Dashed line, $\rho = 0$; solid line, $\rho = 0.1$; dashed-dotted line, $\rho = 0.3$.

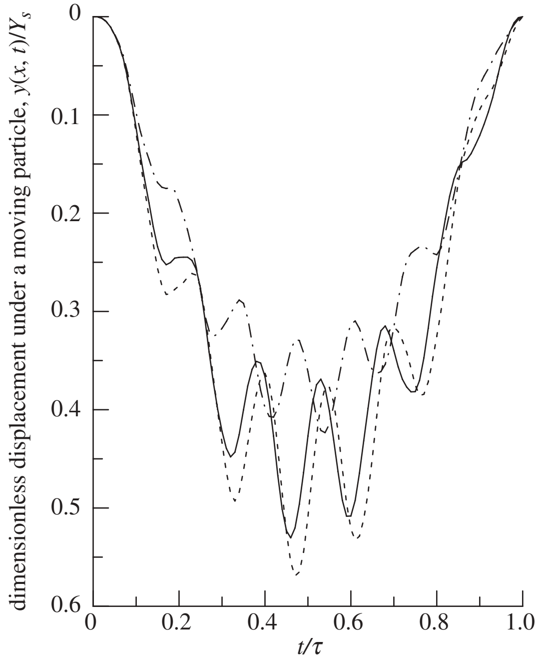

Figure 4. Dimensionless displacement of a SWCNT for nanoparticle delivery at $\alpha = 0.1$, $\rho = 0.1$ and $w = 50$ for different dimensionless times and foundation stiffnesses. Dashed line, $k = 0$; solid line, $k = 10$; dashed-dotted line, $k = 50$.

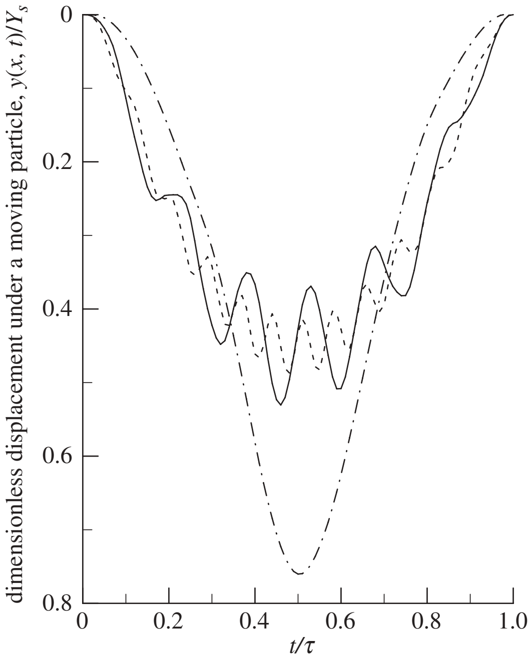

Figure 5. Dimensionless displacement of a SWCNT for nanoparticle delivery at $k=20$, $\rho=0.1$ and $w=50$ for different dimensionless times and velocity ratios of the moving nanoparticle. Dashed line, $\alpha=0.05$; solid line, $\alpha=0.1$; dashed-dotted line, $\alpha=0.5$.

moving nanoparticle. When the value of t/τ is about 0.5, the maximum displacement is obtained because the moving nanoparticle reaches the mid-span of the SWCNT. In addition, it can be seen that the maximum displacement increases with an increasing velocity ratio.

4. Conclusion

The dynamic response of a (10,10) SWCNT conveying a C_{60} fullerene molecule was studied using the non-local elasticity theory. The effects of foundation stiffness, confined stiffness, velocity ratio and travel time on the behaviour were analysed using the Runge–Kutta method. The numerical result was compared with the analytical solution, and the comparison showed a good agreement. According to the analysis, the results showed that increasing the confined stiffness between the delivery nanoparticle and the SWCNT decreased the dynamic displacement of the SWCNT. In addition, increasing the non-local parameter and foundation stiffness also decreased the displacement. However, the maximum displacement increased with increasing velocity ratio.

The authors wish to thank the National Science Council of the Republic of China in Taiwan for providing financial support for this study under projects NSC 98-2221-E-168-019 and NSC 97-2221-E-168-019-MY2.

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