Composite Structures 116 (2014) 254–272

Contents lists available at ScienceDirect

Composite Structures

journal homepage: www.elsevier.com/locate/compstruct

Nanoparticle delivery via stocky single-walled carbon nanotubes: A nonlinear-nonlocal continuum-based scrutiny

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ARTICLE INFO

Article history:
Available online 5 April 2014

Keywords:
Single-walled carbon nanotubes (SWCNTs)
Nanoparticle delivery
Nonlinear vibrations
Nonlocal Timoshenko beam theory
Nonlocal higher-order beam theory
Galerkin approach

ABSTRACT

Excellent mechanical properties plus to the good biocompatibility of single-walled carbon nanotubes (SWCNTs) are offering them as efficient nanodevices for delivering of nanoparticles. Due to the friction between the outer surface of the nanoparticle and the inner surface of the SWCNTs, mass weight of the nanoparticle, and the interactional van der Waals (vdW) forces between the constitutive atoms of the nanoparticle and those of the SWCNT, both longitudinal and transverse waves propagate within the SWCNT. Herein, such vibrations in stocky SWCNTs are of concern in the context of nonlinear-nonlocal continuum theory of Eringen. Based on the Rayleigh, Timoshenko, and higher-order beam theories, the dimensionless equations of motion are constructed and then numerically solved. The effects of the mass weight and velocity of the nanoparticle, radius and length of the SWCNT, the abovementioned vdW forces, and the small-scale parameter on the maximum displacements and forces within the SWCNT are exclusively explored. Additionally, the limitations of both the linear and local analyses for the problem under study are discussed.

1. Introduction

Among various nanoscale materials, carbon nanotube (CNT) is emerging as a new-fangled nanodevice for transferring therapeutic molecules. CNTs [1–4] are the nearly perfect materials for a diverse range of applications. This matter is chiefly related to their exceptional chemical, physical, and mechanical properties [5–8]. CNTs could be functionalized with proteins, nucleic acids, and drugs. Functionalized CNTs exhibit little toxicity to normal biological cells, and are not easily immunogenic. According to the literature [9–13], exploiting functionalized CNTs for drug and protein delivery is going to become one of the most promising applications in the field of nanomedicine. For optimal design of CNTs with such functionalities, understanding the dynamic interactions between moving nanoparticles and such nanostructures is a key prerequisite.

To date, two general aspects of vibrations of CNTs, namely wave propagation/free vibrations [14–19] and forced vibrations [20–22], have been examined. In most of these studies, size-dependent theories have been exploited to explore their vibrations. At the nanoscale, vibrations of each atom influence in the vibrations of its neighboring ones. This fact may become more apparent when the nanostructure is acted upon by a pointed load, high frequency waves, or a shock load. In such cases, the classical continuum mechanics would not be satisfactory since the stress dependency of each point to its neighboring points could not be taken into account at all. To conquer this crucial shortage of the classical continuum mechanics, some advanced or size-dependent theories have been developed in the past century. One of the most renowned theories is the nonlocal continuum mechanics of Eringen [23–26]. In the context of this theory, the size-dependency is considered through a so-called small-scale parameter. This parameter and its kernel function correspond to the state of the stress/strain fields of the neighboring points of a point when that point vibrates. So far, this theory has been extensively employed for the mechanical analysis of CNTs.

From mechanics points of view, when a nanoparticle moves inside the pore of the CNT, some kinds of vibrations will produce within the nanostructure. Generally, the cause of such vibrations are, among other effects, nanoparticle's mass weight, friction, inertial, and existing van der Waals (vdW) forces between the constitutive atoms of the moving nanoparticle and those of the CNT. Recently, the effects of the first two abovementioned issues on the small vibrations of single-walled carbon nanotubes (SWCNTs) were addressed [27–29]. In the latter two works, the inertial effects of both longitudinal and transverse motion of the SWCNT were also incorporated into the suggested models. Further, Kiani

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http://dx.doi.org/10.1016/j.compstruct.2014.03.045
0263-8223/

[30,31] studied small transverse vibrations of double-walled carbon nanotubes, which are acted upon by a moving nanoparticle. To this end, nonlocal classical and shear deformable beam theories were used for modeling the innermost and outermost tubes. In such studies, the inertial effects of the moving nanoparticle were not considered. Recently, Simsek [32] inspected lateral vibration of elastically connected double-carbon nanotubes subjected to a moving nanoparticle. Such investigations were performed in the context of nonlocal continuum theory of Eringen via both an analytical and Galerkin approach. In another work, Simsek [33] studied lateral vibrations of lengthy microbeams subjected to a moving microparticle using a modified couple stress theory. In the two latter works, the inertial and frictional effects of the moving particle were not taken into account. Therefore, as explained in Refs. [28,29], the true dynamic behavior of the nanostructure would not be captured when a moving nanoparticle with high levels of the mass weight and velocity traversed the nanostructure. In all abovementioned works, the effects of the vdW forces were not taken into account. In addition, the predicted results were limited to the linear analyses. Such deficiencies of the previously developed models encouraged the author to investigate more rationally the vibrations of SWCNTs traversed by a moving nanoparticle in the context of nonlinear-nonlocal elasticity accounting for the vdW effect. It is worth mentioning that the produced vibrations within the CNT due to the translocation of the nanoparticle can be also affected by the path of the moving nanoparticle which is traveling on the inner surface of the CNT. Without making our problem more complex than this, to answer to the raised concerns, we restrict our attention to the case where the nanoparticle moves on a straight line.

In this work, both nonlinear longitudinal and transverse vibrations of a stocky SWCNT due to translocation of a nanoparticle through its pore are studied in the framework of the nonlocal continuum theory of Eringen [23–26]. In contrast to the previous studies [27–29,32,33], the effects of the vdW interactional forces between the constitutive atoms of the nanoparticle and those of the SWCNT as well as the geometrically nonlinear behavior of the SWCNT are considered. To this end, the well-known beam models are exploited, and their governing equations accounting for both large deflections and rotations are obtained. By the use of Galerkin method and an efficient finite difference approach, the coupled nonlinear equations of motion for each nonlocal beam model are numerically solved in the spatial and time domains, respectively. The influences of the geometrical properties of the stocky SWCNT, the velocity and mass weight of the nanoparticle, the small-scale parameter, and the vdW interactional force on the maximum displacements and nonlocal forces within the SWCNT due to the movement of a nanoparticle are addressed and discussed.

2. Interactional forces between a moving nanoparticle and a vibrating SWCNT

Consider a SWCNT which is used for translocation of a nanoparticle from its left-hand end to the right-hand one as demonstrated in Fig. 1(a). For continuum-based modeling of the problem, the SWCNT is replaced by an ECS (see Fig. 1(b)). The ECS is a hollow circular isotropic solid whose dominating longitudinal, flexural, and torsional frequencies roughly match with those of the SWCNT. The density, the elasticity modulus, the shearing elastic modulus, the Poisson's ratio, the cross-sectional area, and the moment inertia of the ECS are represented by $\rho_b, E_b, G_b, v_b, A_b$, and I_b, respectively. Moreover, the length of the ECS, l_b, and its wall's thickness, t_b, are, respectively, equal to the length of the SWCNT under study and 0.34 nm [34]. The Cartesian coordinate system is set up such that the x-axis is coincident with the revolution axis of the SWCNT and the z-axis is in the direction of the applied gravitational acceleration, $\mathbf{g} = g\hat{e}_z$ where $\hat{e}_{[.]}$ is the unit vector pertinent to the [.]-axis ([.] = x or y or z). The nanoparticle is assumed to be a rigid solid which is slipping on the lowest points of the inner surface of the SWCNT across a straight line. Thereby, the location of the moving nanoparticle is represented by $(x_M, z_M) = (vt, r_i)$ where t is the time parameter, and the inner and outer radii of the ECS are shown by r_i and r_o, respectively. The weight and the velocity of the moving nanoparticle are assumed to be the constant values Mg and v, respectively. During the course of excitation of the SWCNT, it is supposed that the moving nanoparticle be in contact with the SWCNT. Therefore, the longitudinal and transverse inertial effects of the moving nanoparticle, respectively, denoted by $-M\frac{D^2u_x}{Dt^2}$ and $-M\frac{D^2u_z}{Dt^2}$, should be taken into account in the interactional exerted forces. In these relations, $u_x = u_x(x,y,z,t)$ and $u_z = u_z(x,y,z,t)$ are the longitudinal and transverse displacement fields of the ECS, and $\frac{D^2}{Dt^2}$ is the material derivative of second-order.

By exploiting the Coulomb frictional model, the longitudinal contact force between the moving nanoparticle and the inner surface of the SWCNT is expressed by

$$F_{cx} = \left(\mu_k\left|Mg + F_{vdW} - M\frac{D^2u_z}{Dt^2}\right| - M\frac{D^2u_x}{Dt^2}\right)\delta(x - x_M)\delta(z - z_M)\mathrm{H}(l_b - x_M), \tag{1}$$

where δ and H are the Dirac delta and Heaviside functions, respectively, μ_k is the kinematic friction coefficient, F_{vdW} is the vertical component of the resultant attractive vdW forces between the constitutive atoms of the nanoparticle and those of the SWCNT. The magnitude of such a force could be determined by using the Lenard-Jones potential functions according to the atomic properties of the nanoparticle and those of the rolled graphene (i.e., SWCNT). It is also assumed that F_{vdW} does not alter during the passage of the moving nanoparticle through the SWCNT.

Since the moving nanoparticle would be in contact with the inner surface of the SWCNT, and the lonely externally applied force on the moving nanoparticle is the mass weight force, the transverse component of the interactional force could be written as,

$$F_{cz} = M\left(g - \frac{D^2u_z}{Dt^2}\right)\delta(x - x_M)\delta(z - z_M)\mathrm{H}(l_b - x_M). \tag{2}$$

In this work, the longitudinal and transverse vibrations of the SWCNT due to slipping motion of the nanoparticle are of concern. Therefore, appropriate beam models can be employed for prediction of the dynamical deformation of the ECS subjected to the contact forces expressed by Eqs. (1) and (2). Herein, three well-known beam theories, namely Rayleigh, Timoshenko, and higher-order beam theories, are exploited, and it is aimed to construct their nonlinear governing equations for the problem under study. In such beam models, the longitudinal and transverse displacements are approximated by the midspan displacements and deformation angle as,

$$\begin{aligned}
&u_x^R(x,y,z,t) = u^R(x,t) - zw_x^R(x,t),\ u_z^R(x,y,z,t) = w^R(x,t),\\
&u_x^T(x,y,z,t) = u^T(x,t) + z\theta^T(x,t),\ u_z^T(x,y,z,t) = w^T(x,t),\\
&u_x^H(x,y,z,t) = u^H(x,t) - z\psi^H(x,t) - \alpha z^3\left(-\psi^H + w_x^H\right),\ u_z^H(x,y,z,t) = w^H(x,t),
\end{aligned} \tag{3}$$

where $\alpha = 1/(3r_o^2), u^R/w^R, u^T/w^T$, and u^H/w^H denote the longitudinal/transverse displacements of the Rayleigh, Timoshenko, and higher-order beam theories, respectively. Additionally, θ^T and ψ^H in order represent the deflection angles of the Timoshenko and higher-order beam models. By introducing Eq. (3) to Eqs. (1) and (2), the longitudinal interactional forces between the moving