Nonlinear vibration properties of a zigzag single-walled carbon nanotube embedded in a polymer matrix

Abderrahmane Besseghier\textsuperscript{1,2}, Houari Heireche\textsuperscript{1,3}, Abdelmoumen Anis Bousahla\textsuperscript{1,3,4}, Abdelouahed Tounsi\textsuperscript{*1,3,4,5} and Abdelnour Benzair\textsuperscript{1,3}

\textsuperscript{1}Laboratoire de Modélisation et Simulation Multi-échelle, Département de Physique, Faculté des Sciences Exactes, Département de Physique, Université de Sidi Bel Abbès, Algeria
\textsuperscript{2}Centre Universitaire de Tissemsilt, Algeria
\textsuperscript{3}Algerian National Thematic Agency of Research in Science and Technology (ATRST), Algeria
\textsuperscript{4}Material and Hydrology Laboratory, Faculty of Technology, Civil Engineering Department, University of Sidi Bel Abbes, Algeria
\textsuperscript{5}Laboratoire des Structures et Matériaux Avancés dans le Génie Civil et Travaux Publics, Faculté de Technologie, Département de Génie Civil, Université de Sidi Bel Abbès, Algérie

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Abstract. In the current study, the nonlinear vibration properties of an embedded zigzag single-walled carbon nanotube (SWCNT) are investigated. Winkler-type model is used to simulate the interaction of the zigzag SWCNTs with a surrounding elastic medium. The relation between deflection amplitudes and resonant frequencies of the SWCNT is derived through harmonic balance method. The equivalent Young’s modulus and shear modulus for zigzag SWCNT are derived using an energy-equivalent model. The amplitude – frequency curves for large-amplitude vibrations are graphically illustrated. The simulation results show that the chirality of zigzag carbon nanotube as well as surrounding elastic medium play more important roles in the nonlinear vibration of the single-walled carbon nanotubes.

Keywords: zigzag carbon nanotube; nonlinear vibration; harmonic balance method

1. Introduction

In the last few years, carbon nanotubes (CNTs) have attracted extensive research activities due to their exceptional mechanical, physical, chemical and thermal properties. CNTs were first discovered by Iijima (1991) in 1991. To make the full potential applications of CNTs, understanding their mechanical behavior is essential and has become a hot topic. In particular, considerable efforts have been devoted to understand the mechanical behavior of CNTs recently (Fu \textit{et al.} 2006, Yoon \textit{et al.} 2003, Amin \textit{et al.} 2009, Mahdavi \textit{et al.} 2009, Heireche \textit{et al.} 2008a, b, c, Tounsi \textit{et al.} 2008, Murmu and Adhikari 2011, Tounsi \textit{et al.} 2013a, b, Pradhan and Mandal 2013).

During the past decade, several methods have been pursued to investigate and characterize the mechanical behavior of CNTs. Since experiment is difficult to conduct on nanoscale and

*Corresponding author, Professor, E-mail: tou_abdel@yahoo.com

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molecular dynamics simulation is not time-and cost-effective. Thus, elastic continuum modeling of nanostructures has become a very important issue (Behfar et al. 2005, Popov et al. 2000, Sohi and Naghdabadi 2007, Sun and Liu 2008, Bessegghier et al. 2011, Gafour et al. 2006). These studies, among others, have demonstrated the powerfulness of continuum mechanics, i.e., using simple formula offered by these continuum models, key parameters that affect the mechanical behavior of CNTs can be easily discovered to predict new physical phenomena. Most existing studies in literature are linear analysis on the vibrations of CNTs. However, there are much fewer studies on the nonlinear mechanical behavior of CNTs. Fu et al. (2006) investigated the nonlinear free vibration of embedded multi-walled CNTs considering inter-tube radial displacement and the related internal degrees of freedom. Xu et al. (2006) studied the vibration of a double-walled CNTs induced by nonlinear interlayer van der Waals (vdW) forces which were described as the nonlinear function of interlayer spacing. Nonlinear vibrations of nanotubes have been studied also in (Fu et al. 2006) in the case of a single nanotube and in (Fu et al. 2009) in the case of DWCNTs where geometric nonlinearity and simply supported boundary conditions were considered.

The literature lacks a comprehensive study on nonlinear free vibration of embedded CNTs with considering the chirality effect. The present work tries to fill this gap where the effect of chirality on the nonlinear vibration response of embedded zigzag CNTs is studied.

In this paper, based on the continuum mechanics and a single-elastic beam model, the nonlinear free vibration analysis of embedded zigzag CNT is investigated. The novelty of this present work in contrast to Fu et al. (2006) is that the chirality of zigzag carbon nanotube is included in the theoretical formulation. The equivalent Young’s modulus for zigzag SWCNT is derived using an energy-equivalent model (Wu et al. 2006, Zidour et al. 2012, Baghdadi et al. 2014, Semmah et al. 2014, Zidour et al. 2014, Benguediab et al. 2014, Naceri et al. 2011, Tokio, 1995). The obtained results in this work can provide useful guidance for the study and design of the next generation of nanodevices that make use of the thermal vibration properties of zigzag carbon nanotubes.

2. Basic equations

Consider a zigzag CNT of length $L$, Young’s modulus $E_z$, density $\rho$, cross sectional area $A$, and cross-sectional inertia moment $I$, embedded in an elastic medium (as shown in Fig. 1) with constant $k$ determined by the material constants of the surrounding medium. Assume that the displacement of zigzag CNT along $x$ direction is $u(x, t)$, and the displacement along $z$ direction is
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Fig. 2 (a) An armchair, (b) a zigzag and (c) a chiral nanotube and (d) a graphene being rolled into a cylinder

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$w(x, t)$ in terms of the spatial coordinate $x$ and the time variable $t$. The free vibration equation of embedded zigzag CNT considering the geometric nonlinearity of the structure is (Fu et al. 2006)

$$E_z I \frac{d^4 w}{dx^4} + \rho A \frac{d^2 w}{dt^2} + k w = \left[ \frac{E_z A}{2L} \left( \frac{d w}{dx} \right)^2 \right] \frac{d^2 w}{dx^2}$$

(1)

where the equivalent Young’s modulus of a zigzag CNT is expressed using an energy-equivalent model (Wu et al. 2011, Zidour et al. 2012) as follows

$$E_z = \frac{4\sqrt{3}KC}{9Ct_z + 4Ka_z^2t_z (\lambda_{z1}^2 + 2\lambda_{z2}^2)}$$

(2)

and $K$ and $C$ are the force constants. $t_z$ is the thickness of the nanotube and the parameters $\lambda_{z1}$ and $\lambda_{z2}$ are given by

$$\lambda_{z1} = \frac{-3\sqrt{4 - 3\cos^2(\pi/2n)} \cos(\pi/2n)}{8\sqrt{3} \cdot 2 \sqrt{3} \cos^2(\pi/2n)}$$

$$\lambda_{z2} = \frac{12 - 9\cos^2(\pi/2n)}{16\sqrt{3} \cdot 4\sqrt{3} \cos^2(\pi/2n)}$$

(3)

Fig. 2 shows the lattice indices of translation $(n, m)$ along with the base vectors. The radius of the zigzag nanotube $(n, 0)$ in terms of the chiral vector components can be obtained from the relation (Wu et al. 2006)

$$R = \frac{na_z}{2\pi} \sqrt{3},$$

(4)

where $a_z$ is the length of the carbon–carbon bond which is $1.42\text{Å}$ and $n$ is the index of translation, which decide the structure around the circumference.

For a simply supported nanotube at the two ends, the deflection $w(x, t)$ may be given as
Fig. 3 Effect of the chirality number \((n)\) on nonlinear amplitude frequency response curves of zigzag SWCNT for different Winkler modulus parameters: (a) \(k=0\); (b) \(k=10^7\), (c) \(k=10^8\), (d) \(k=10^9\)
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By substituting Eq. (5) into Eq. (1), the nonlinear differential equation for the time function \( W(t) \) can be obtained as follows

\[
\frac{d^2W}{dt^2} + \left[ \frac{\pi^4 E I}{L^4 \rho A} + \frac{k}{\rho A} \right] W + \frac{\pi^4 E I}{4L^4 \rho} W^3 = 0
\]

(6)

Introducing the dimensionless parameters

\[
r = \sqrt{I/A}, \quad a = W/r, \quad \omega_l = \frac{\pi^2}{L^2} \sqrt{\frac{E I}{\rho A}}, \quad \omega_k = \sqrt{\frac{k}{\rho A}}, \quad \tau = \omega t
\]

(7)

By substituting Eq. (7) into Eq. (6), the dimensionless nonlinear vibration governing equation is given as

\[
\left( \frac{\omega}{\omega_l} \right)^2 \frac{d^2 a}{d\tau^2} + \left[ 1 + \left( \frac{\omega}{\omega_l} \right)^2 \right] a + \alpha a^3 = 0
\]

(8)

where \( \alpha = 0.25 \). Eq. (8) is the famous Duffing equation. The method of harmonic balance is adopted to find an analytical solution of good accuracy to the problem.

3. Numerical results and discussion

The material and geometric parameters considered here for a zigzag CNT are \( \rho = 1300 \text{ kg/m}^3 \)
Fig. 4 Effect of the Winkler modulus parameters (k) on nonlinear amplitude frequency response curves of zigzag SWCNT with n=3

(Pantano et al. 2003), L=45 nm, the outside diameter is d₁=3 nm, the inside diameter is d₀=2.32 nm. The linear free vibration frequency is assumed to be ωₗ in Eq. (8), and \( \omega_0^2 = \omega_l^2 + \omega_b^2 \).

The effect of the chirality number on the amplitude-frequency response curves for a zigzag SWCNT with different Winkler modulus parameters k are shown in Fig. 3. From the figure it is observed that there is significant influence of the chirality number on the amplitude-frequency response curves for an embedded zigzag SWCNT (k≠0). However, this effect is not obvious for a zigzag SWNT without a surrounding elastic medium (Fig. 3(a)). Further, it can be seen that the effect of the chirality number, is more significant for lower values of index of translation n and higher Winkler modulus parameters.

The effect of the Winkler modulus parameters k on the amplitude-frequency response curves of the zigzag SWCNT (n=3) are shown in Fig. 4. From the results illustrated in Fig. 4, it is noted that the Winkler modulus parameter k of surrounding elastic medium has a pronounced effect on the nonlinear amplitude frequency response curves of zigzag SWCNT. It can be also seen that the nonlinear free vibration frequency of nanotubes rises rapidly with the increment of the vibration amplitude when the stiffness of medium is relatively small (say \( k<10^7 \) N/m² (Yoon et al. 2003, Lanir and Fung 1972)), in which case the variation of spring constant k has little effect on the response curves of zigzag SWCNT. Thus, the effect of surrounding elastic medium can be neglected when the medium is flexible (such as a polymer medium).

4. Conclusions

In this article, the nonlinear vibration properties of embedded zigzag SWCNT are investigated on the basis of the continuum mechanics and the single-elastic beam model. Theoretical formulations include the Winkler modulus parameter and the chirality of zigzag SWCNT. According to this work, the results showed the dependence of the nonlinear vibration characteristics on the chirality of zigzag SWCNT and the surrounding elastic medium. The
important conclusions that emerge from this paper can be summarized as follows:

• The nonlinear free vibration of zigzag SWCNT is influenced considerably by surrounding elastic medium.
• The nonlinear vibration characteristics are affected significantly by the chirality of zigzag SWCNT.
• The effect of the chirality of zigzag SWCNT on the amplitude frequency response curves is significantly felt when the stiffness of elastic medium becomes large enough.


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