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Higher order nonlocal strain gradient approach for wave characteristics of carbon nanorod

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Abstract. In this paper an attempt is made to study the wave dispersion characteristics of a carbon nanorod through second, fourth, sixth and eighth order nonlocal strain gradient models. Expressions are derived for both wave number and wave speeds of the nanorod. The wave characteristics of the nanorod obtained from the nonlocal strain gradient models are compared with the classical continuum model. From these models it is observed that sixth order strain gradient model gives the better approximation than the second and fourth order strain gradient models for dynamic analysis. The second and sixth order strain gradient models gave critical wave number at a certain wave frequency, which does not exist in fourth and eight order strain gradient models.

Keywords: nonlocal elasticity, nanorod, wave propagation, critical wave number.

1 Introduction

A nanostructure is an object in which at least one of its dimension is in nanoscale (lessthan 100 nm). The nanostructures including nanotube, nanobeam and nanorod etc., have become important potential designs in many engineering applications. A great deal of research [1–3] in these areas shows that, one can study the mechanical, electrical, chemical and thermal conductivity properties of nanostructures using bending, vibration and wave propagation through nanostructures. All these studies are under a broad area known as nano-electromechanical systems (NEMS). Mechanical behavior such as vibration, buckling analysis, bending phenomena of carbon nanorods and nanotubes are generally characterized as micro-electromechanical systems (MEMS) [4–7]. Carbon nanorods not only possess beam like structures but also have size effect in which bending stiffness and young modulus are diameter dependent [8].

The nonlocal elasticity theory used in this paper, was first developed by Eringen [9] and his associates. It assumes that the stress at a reference point in the elastic continuum is a function of elastic strain field at every point in that model. This theory is based on

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the atomic theory of lattice dynamics and on phonon dispersions. Recently several authors [10–15] worked on the wave propagation in carbon nanotubes using strain gradient models. The effect of nanoscale on the frequency, phase velocity and group velocities and several other properties have been studied in certain special strain gradient models.

The main objective of this paper is to present a nonlocal higher order strain gradient model for studying transverse wave propagation in carbon nanorod using nonlocal elasticity theory. The nonlocal theory is applied to obtain second, fourth, sixth and eighth order strain gradient models. The effect of wave numbers on wave frequency, phase velocity and group velocity has been studied numerically for each strain gradient model. The critical wave number is observed for second and sixth strain gradient model. However, the critical wave number is not observed in case of fourth and eighth order strain gradient models. The strain gradient models of different orders explains the heterogeneity of the particular nonlocal elastic continuum [16, 17].

2 Basic equations of nonlocal elasticity

The nonlocal elastic stress field theory concerns the state of stress at a reference point r' within domain. The nonlocal stress depends not only on the strain at that location but also on the strain at all other points within the domain in a diminishing influence away from the reference location. The nonlocal elastic field theory for homogeneous and isotropic solids is described using the following basic equations [11, 12, 14]:

$$\sigma_{ij,i} + \rho(f_j - \ddot{u}_j) = 0, \tag{1}$$

$$\begin{aligned} \sigma_{ij}(r) &= \int_v \alpha\bigl(|r' - r|, \tau\bigr)\sigma'_{ij}(r')\,\mathrm{d}v(r'), \\ \sigma'_{ij}(r') &= \lambda e_{kk}(r')\delta_{ij} + 2\mu e_{ij}(r'), \\ e_{ij}(r') &= \frac{1}{2}\left[\frac{\partial u_j(r')}{\partial r'_i} + \frac{\partial u_i(r')}{\partial r'_j}\right], \end{aligned} \tag{2}$$

where $\sigma_{ij}(r)$, ρ, f_j and u_j are the nonlocal stress tensor, mass density, body force density and displacement vector at time t respectively at a reference point r in the body, while $\ddot{u}_j$, the second derivative of u_j with respect to time t is the acceleration vector at r, and the indices i, j take the values 1 (or) 1, 2 (or) 1, 2, 3 depending on the dimensions of the body. The linear relationship between the local stress tensor $\sigma'_{ij}(r')$ and classical strain tensor $e_{ij}(r')$ at any arbitrary point r' is shown in Eq. (2). λ, μ are the Lame constants and δ_{ij} is the Kronnecker delta. The nonlocal kernal function denoted by $\alpha(|r' - r|, \tau)$ depends on the Euclidean distance $|r' - r|$ between the reference point r and the arbitrary point r' and on the dimensionless nanolength scale τ. The dimensionless nanolength scale τ is described in [2] as

$$\tau = \frac{e_0 a}{L}.$$

Here a is the internal characteristic length (ex. lattice parameter, C–C bond length, granular distance), and L is an external characteristic length (ex. crack length, wave length etc.)

of the nanorod. Also, we take e_0 as an nonlocal scaling parameter, which is assumed to be constant appropriate to continuum model. The classical Hooke's law for uniaxial stress in one dimension can be determined by using a nonlocal stress-strain relation [11] from (1) as

$$\sigma(x) - (e_0 a)^2 \frac{\mathrm{d}^2\sigma(x)}{\mathrm{d}x^2} = E\epsilon(x), \tag{3}$$

where E is the Young's modulus and $\sigma(x)$, $\epsilon(x)$ are respectively the normal stress and normal strain in the axial direction of the nonlocal nanorod. As a limiting case, if the nanoscale $e_0 a$ tends to zero the nonlocal effect can be neglected and the nonlocal stress σ approaches to that of the corresponding classical stress $\sigma'(x) = E\epsilon(x)$. It is noted that the above equation (3) is a one dimensional ordinary differential equation.

3 Nonlocal strain gradient models

For simplicity and standardization, we introduce the dimensionless variable $\bar{x} = x/L$ and $\tau = e_0 a/L$, where L is the the length of nanorod. The solution of nonlocal stress strain relation (3) in terms of strain gradient can be expressed as

$$\sigma(x) = E\left[\epsilon(x) + \sum_{n=1}^{\infty} \tau^{2n} \frac{\mathrm{d}^{2n}\epsilon(x)}{\mathrm{d}\bar{x}^{2n}}\right]. \tag{4}$$

By taking $n = 1, 2, 3, 4$ in the above equation (4) we obtain the second, fourth, sixth and eighth order strain gradient models, respectively.

4 Governing partial differential equation of the wave propagation

For a given nanorod, the displacement field and strain gradient are given by

$$u = u(\bar{x}, t), \qquad \epsilon = \frac{\partial u}{\partial \bar{x}},$$

where $\bar{x}$ is the axial co-ordinate, $u = u(\bar{x}, t)$ is the axial displacement, t is the time variable. We represent the area of cross section of the nanorod of length L as A.

The potential energy (U) and kinetic energy (K) of the nanorod for the second order strain gradient model are given by

$$U = \frac{1}{2}\int_v \sigma(x)\epsilon(x)\,\mathrm{d}v = \frac{E}{2}\int_v \left[\epsilon(x) + \tau^2 \frac{\partial^2\epsilon(x)}{\partial x\bar{x}^2}\right]\mathrm{d}v, \qquad K = \frac{E}{2}\int_v \rho\left[\frac{\partial u(\bar{x}, t)}{\partial t}\right]^2 \mathrm{d}v.$$

By applying Hamilton's principle

$$\delta\int_{t_1}^{t_2} (K - U)\,\mathrm{d}t = 0. \tag{5}$$

Expanding (5), the nonlocal partial differential equation for the nanorod from the second order strain gradient model obtained as

$$EA\tau^2\frac{\partial^4 u(\bar{x},t)}{\partial\bar{x}^4}+EA\frac{\partial^2 u(\bar{x},t)}{\partial\bar{x}^2}-\rho A\frac{\partial^2 u(\bar{x},t)}{\partial t^2}=0. \tag{6}$$

This is a fourth order partial differential equation. The classical wave equation can be obtained by taking $\tau = 0$ in (6). By applying the above procedure the corresponding partial differential equations of fourth, sixth and eight order strain gradient models are

$$EA\tau^4\frac{\partial^6 u(\bar{x},t)}{\partial\bar{x}^6}+EA\tau^2\frac{\partial^4 u(\bar{x},t)}{\partial\bar{x}^4}+EA\frac{\partial^2 u(\bar{x},t)}{\partial\bar{x}^2}-\rho A\frac{\partial^2 u(\bar{x},t)}{\partial t^2}=0, \tag{7}$$

$$\begin{aligned}&EA\tau^6\frac{\partial^8 u(\bar{x},t)}{\partial\bar{x}^8}+EA\tau^4\frac{\partial^6 u(\bar{x},t)}{\partial\bar{x}^6}+EA\tau^2\frac{\partial^4 u(\bar{x},t)}{\partial\bar{x}^4}+EA\frac{\partial^2 u(\bar{x},t)}{\partial\bar{x}^2}\\&\quad-\rho A\frac{\partial^2 u(\bar{x},t)}{\partial t^2}=0,\end{aligned} \tag{8}$$

$$\begin{aligned}&EA\tau^8\frac{\partial^{10} u(\bar{x},t)}{\partial\bar{x}^{10}}+EA\tau^6\frac{\partial^8 u(\bar{x},t)}{\partial\bar{x}^8}+EA\tau^4\frac{\partial^6 u(\bar{x},t)}{\partial\bar{x}^6}+EA\tau^2\frac{\partial^4 u(\bar{x},t)}{\partial\bar{x}^4}\\&\quad+EA\frac{\partial^2 u(\bar{x},t)}{\partial\bar{x}^2}-\rho A\frac{\partial^2 u(\bar{x},t)}{\partial t^2}=0.\end{aligned} \tag{9}$$

5 Analytical solution of the models

The analytical solution of second and fourth strain gradient models in terms of displacement field u are obtained by using the uniaxial equilibrium equation $\partial\sigma/\partial x = 0$ and the kinematic relation $\varepsilon = \partial u/\partial x$. Thus, the analytical solutions of second and fourth order strain gradient models are

$$\begin{aligned}u&=(c_1+c_2\bar{x})+c_3\cos\frac{\bar{x}}{\tau L}+c_4\sin\frac{\bar{x}}{\tau L}\\&=(c_1+c_2\bar{x})+\mathrm{e}^{\bar{x}/(2(\tau L)^2)}\left[(c_3+c_4\bar{x})\cos\frac{\sqrt{3}}{2(\tau L)^2}+(c_5+c_6\bar{x})\sin\frac{\sqrt{3}}{2(\tau L)^2}\right].\end{aligned}$$

Here the arbitrary constants c_j (for $j = 1, 2, \dots, 6$) are determined by using the Clamped boundary conditions $\Delta u = 0$ and $\partial\Delta u/\partial\bar{x} = 0$ at both the ends $x = 0$, $x = L$. The similar solutions can be easily obtained for remaining strain gradient models.

6 The wave characteristics of the nanorod

The ultrasonic wave dispersion characteristics in nanorod can be analyzed by assuming a harmonic type of wave solution for the displacement field $u(\bar{x},t)$, which can be expressed in complex form as

$$u(\bar{x},t)=\hat{u}(\bar{x},\omega)\mathrm{e}^{-\mathrm{i}(\bar{k}\bar{x}-\omega t)}, \tag{10}$$

where $\hat{u}(\bar{x}, \omega)$ is the amplitude of the longitudinal displacement, k is the wave number, $\bar{k} = kL$ and ω is the angular frequency of the wave motion. On substitution of Eq. (10) in the nonlocal partial differential equation of nanorod obtained from the second order strain gradient model (6), the dispersive relation is

$$(\tau\bar{k})^2\bar{k^4} - \bar{k}^2 + \eta^2\omega^2 = 0, \tag{11}$$

where $\eta = \sqrt{\rho/E}$. The wave frequency from the dispersive relation (11) can be expressed as

$$\omega = \frac{\bar{k}}{\eta}\sqrt{1 - (\tau\bar{k})^2},$$

clearly, the wave frequency is a function of wave number k, the nonlocal parameter τ and the material properties of the carbon nanorod. The phase velocity (p_2) and group velocity (g_2) of the second order strain gradient model of the nanorod derived as

$$p_2 = \frac{\omega}{\bar{k}} = \frac{1}{\eta}\sqrt{1 - (\tau\bar{k})^2}, \qquad g_2 = \frac{\partial\omega}{\partial\bar{k}} = \frac{1 - 2(\tau\bar{k})^2}{\eta\sqrt{1 - (\tau\bar{k})^2}}.$$

By taking nonlocal parameter $\tau = 0$ we get $p_2 = g_2 = 1/\eta = \sqrt{E/\rho}$, which is same as that of classical continuum model.

The above procedure is repeated to the fourth order strain gradient model (7), which gives the dispersive relation as

$$-(\tau\bar{k})^4\bar{k^6} + \tau\bar{k})^2\bar{k^4} - \bar{k}^2 + \eta^2\omega^2 = 0.$$

The wave frequency from the above relation is

$$\omega = \frac{\bar{k}}{\eta}\sqrt{1 - (\tau\bar{k})^2 + (\tau\bar{k})^4}.$$

Similarly phase velocity (p_4) and group velocity (g_4) for fourth order strain gradient model are obtain as

$$p_4 = \frac{1}{\eta}\sqrt{1 - (\tau\bar{k})^2 + (\tau\bar{k})^4}, \qquad g_4 = \frac{1 - 2(\tau\bar{k})^2[1 - (\tau\bar{k})^2]}{\eta\sqrt{1 - (\tau\bar{k})^2 + (\tau\bar{k})^4}}.$$

From the sixth order strain gradient model equation (8), the dispersive relation is

$$(\tau\bar{k})^6\bar{k^8} - (\tau\bar{k})^4\bar{k^6} + \tau\bar{k})^2\bar{k^4} - \bar{k}^2 + \eta^2\omega^2 = 0. \tag{12}$$

The wave frequency is

$$\omega = \frac{\bar{k}}{\eta}\sqrt{1 - (\tau\bar{k})^2 + (\tau\bar{k})^4 - (\tau\bar{k})^6},$$

the phase (p_6) and group (g_6) velocities for sixth order strain gradient model are

$$p_6 = \frac{1}{\eta}\sqrt{1 - (\tau\bar{k})^2 + (\tau\bar{k})^4 - (\tau\bar{k})^6}, \qquad g_6 = \frac{1 - (\tau\bar{k})^2[2 - 3(\tau\bar{k})^2 + 4(\tau\bar{k})^4]}{\eta\sqrt{1 - (\tau\bar{k})^2 + (\tau\bar{k})^4 - (\tau\bar{k})^6}}.$$

From the eighth order strain gradient model (9), the dispersive relation and wave frequency as well as the phase (p_8) and group (g_8) velocities may be written as

$$-(\tau\bar{k})^8\bar{k^{10}} + (\tau\bar{k})^6\bar{k^8} - (\tau\bar{k})^4\bar{k^6} + (\tau\bar{k})^2\bar{k^4} - \bar{k}^2 + \eta^2\omega^2 = 0,$$

$$\omega = \frac{\bar{k}}{\eta}\sqrt{1 - (\tau\bar{k})^2 + (\tau\bar{k})^4 - (\tau\bar{k})^6 + (\tau\bar{k})^8},$$

$$p_8 = \frac{1}{\eta}\sqrt{1 - (\tau\bar{k})^2 + (\tau\bar{k})^4 - (\tau\bar{k})^6 + (\tau\bar{k})^8}, \tag{13}$$

$$g_8 = \frac{1 - (\tau\bar{k})^2[2 - 3(\tau\bar{k})^2 + 4(\tau\bar{k})^4 - 5(\tau\bar{k})^5]}{\eta\sqrt{1 - (\tau\bar{k})^2 + (\tau\bar{k})^4 - (\tau\bar{k})^6 + (\tau\bar{k})^8}}. \tag{14}$$

On substitution of $\tau = 0$ in Eqs. (13) and (14) gives $p_8 = g_8 = 1/\eta = \sqrt{E/\rho}$. Also is can be observe that when $\tau = 0$, the wave speeds obtained from fourth, sixth and eighth order strain gradient models are equal to the wave speeds in the classical carbon nanorod.

7 Critical wave number

For the dispersive relations (11) and (12), the critical wave number can be computed by making the wave frequency $\omega = 0$. It is interesting to observe that the second order strain gradient model (11) and sixth order strain gradient model (12) gives the critical wave number as

$$k_{cr} = \frac{1}{\tau} = \frac{L}{e_0 a}.$$

The critical wave number is purely a function of dimensionless length scale τ. However, from the dispersive relations of fourth and eighth strain gradient models it is interesting to observe that these models do not possess a critical wave number, this shows that the same effect of nonlocal parameter τ and the higher order strain gradient models. This variations can be clearly observed in figures shown in the next section.

8 Numerical results and discussion

In the present discussion, we consider a single walled homogenous and isotropic carbon nanorod of diameter $d = 5$ nm, length $L = 10$ nm. The material properties of carbon nanorod are taken as Young's modulus $E = 0.72$ TPa, density $\rho = 2.38$ g/cm^3.

The dispersion relation obtained from the classical continuum model shows that the waves in nanorod are non dispersive i.e., the wave number has a linear relation with the wave frequency or the phase or group speeds are constant. The strain gradient models shows that the waves in nanorod are dispersive in nature. It can be seen that the sixth and eight order strain gradient models gives a better approximations over than the second and fourth order strain gradient models. The second and sixth order strain gradient model behave in similar manner while fourth and eighth order strain gradient models behave as similar but different from that of second and fourth order strain gradient models.

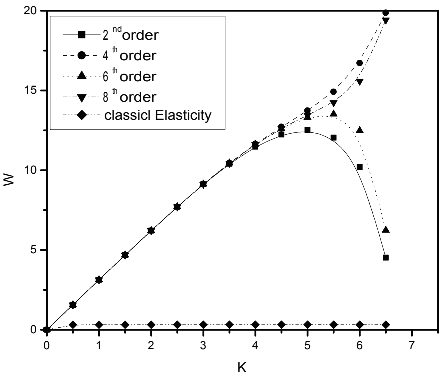

Fig. 1. Effect of nonlocal scaling parameter on wave number dispersion on carbon nanorod.

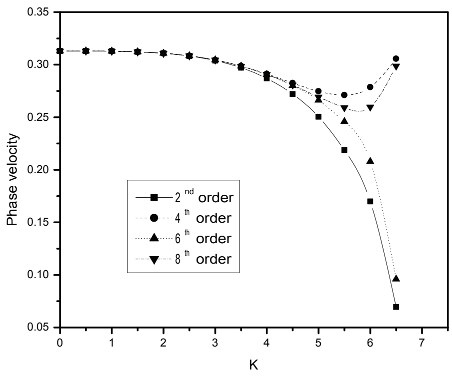

Fig. 2. Effect of nonlocal scaling parameter on phase speed dispersion on carbon nanorod.

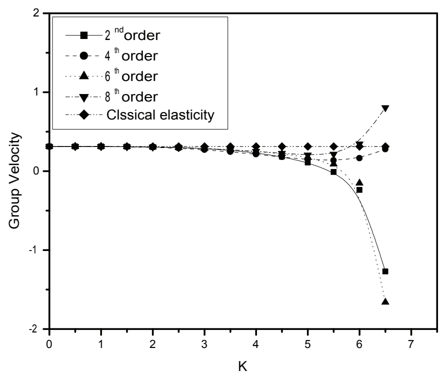

Fig. 3. Effect of nonlocal scaling parameter on group speed dispersion on carbon nanorod.

Figure 1 shows that as the wave number (k) increases, frequency (ω) increases in case of fourth and eighth order strain gradient models. However in case of second and sixth strain gradient models the wave frequency (ω) decreases after reaching the critical point.

From Figs. 2 and 3, it can be observe that the phase velocity and group velocity obtained from the second and sixth order strain gradient models become zero at a particular wave frequency. It also can be seen that in fourth and eighth order strain gradient models, both the group and phase velocities increases along with the wave number. In case of second and sixth strain gradient models the waves cannot propagate to the continuum for the wave number greater than critical wave number.

9 Conclusions

In this paper, the nonlocal higher order strain gradient model for studying transverse wave propagation in carbon nanorod using nonlocal elasticity theory is presented. The effect of wave numbers on wave frequency, phase velocity and group velocity has been studied numerically for each strain gradient model. From the present study that the critical wave number decreases with the increase of scaling parameter. The behavior of wave propagation through nanorods with second and sixth order strain gradient models will be quite different when compare to fourth and eighth order strain gradient models. The wave propagation through nanorods for higher order strain gradient models will behave differently approaches when compared to classical models. The critical wave number is obtained in Second and sixth strain gradient model but it is not observed in case of fourth and eighth order strain gradient models.

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