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# WAVE PROPAGATION IN CARBON NANOTUBES: NONLOCAL ELASTICITY-INDUCED STIFFNESS AND VELOCITY ENHANCEMENT EFFECTS

C. W. LIM AND Y. YANG

We establish the physics and understanding of nonlocal nanoscale wave propagation in carbon nanotubes (CNTs) based on nonlocal elastic stress field theory. This is done by developing an analytical nonlocal nanotube model based on the variational principle for wave propagation in CNTs. Specifically, we successfully derive benchmark governing equations of motion for analyzing wave propagation based on an analytical nonlocal shear deformable model. The physical insights of the analytical nonlocal stress model are presented through examples. Analytical solutions with significant observation of wave propagation have been predicted and the prediction compares favorably with molecular dynamic simulations. Qualitative comparisons with other non-nonlocal approaches, including the strain gradients model, the couple stress model and experiments, justify the stiffness enhancement conclusion as predicted by the new nonlocal stress model. New dispersion and spectrum relations derived using this analytical nonlocal model bring an important focus onto the critical wavenumber: stiffness of CNTs and wave propagation are enhanced below the critical wavenumber, while beyond that a sharp decrease in wave propagation is observed. The physics of nanoscale wave propagation in nanotubes are further illustrated by relating the nanoscale and the phase velocity ratio.

## 1. Introduction

The discovery of carbon nanotubes (CNTs) in the early 1990s [Iijima 1991] created enormous interest among physicists, chemists and engineers, thanks to their unusual mechanical, electrical, electronic, chemical and thermal conductivity properties [Iijima 1991; Treacy et al. 1996; Ajayan and Zhou 2001; Ball 2001; Baughman et al. 2002].

There are many cross disciplinary research works in analytical and computational approaches for CNTs which consider their physical, electrical, chemical and engineering characteristics. There have been comparatively fewer experimental studies on CNTs because at such length scale it is extremely difficult to control, operate precisely and test the specimen. Furthermore, many experimental reports disagree considerably in the measurement of various properties under slightly different test environment. To complement such shortages, a number of continuum and discrete models for CNTs have been proposed.

Molecular dynamic (MD) simulation is the most common computational approach for analyzing CNTs. Using this method, every molecule is single-walled or double-walled CNTs is modeled as a discrete point mass the web of thousands or millions of point masses are constituted in a structured configuration

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through intermolecular bonds and forces [Brenner et al. 2002; Liew et al. 2004a; Liew et al. 2004b; Liew et al. 2005; Kitipornchai et al. 2005]. Although MD has been successful to a certain extent and in a number of cases of study, it is bounded by computational, memory and other hardware constraints. This approach has been restrictive in many cases when very many molecules are required in a nanostructural model. Any premature breakdown of computation due to either algorithmic flaw itself or external power interruption may require the jobs to be restarted or repeated. Hence, the MD analysis has been common for moderate configurations of CNTs and restrictive for complicated CNTs.

To complement MD simulations, continuum elastic models of CNTs have been developed and applied in a number of studies since the middle of 1990s. The early models involve the classical beam, tube or shell models coupled with appropriate molecular potentials to study the mechanical characteristics such as static bending and buckling [Yakobson et al. 1996; Ru 2000a; Ru 2000b; Parnes and Chiskis 2002; Han et al. 2005] and dynamic vibration and wave propagation [Zhang et al. 2005; Yoon et al. 2005; Natsuki et al. 2005; Wang et al. 2006a; Wang and Varadan 2006] of CNTs. The study of wave propagation in CNTs has attracted intensive attention in research because many crucial physical properties such as electrical conductance, optical transition and some dynamic behavior of CNTs are very sensitive to the presence of wave [Zhang et al. 2005]. Among the early studies, the continuum shell model was developed by Natsuki [Natsuki et al. 2005] to predict wave propagation in single-walled CNT embedded in an elastic medium. [Wang and Varadan 2006] applied the elastic beam theory to study the wave characteristics of single-walled and double-walled CNTs base on both thin and thick beam models.

Another continuum model applicable to the analysis of CNTs is the nonlocal elasticity stress field theory which was first proposed in [Eringen and Edelen 1972; Eringen 1972a; 1972b; 1983; 2002]. According to this theory, the stress at a point within a continuous domain with nanoscale effects is dependent not only on the strain at that point but it is also significantly influenced by the stress of all points in the domain through a nonlocal modulus in an integral sense. With such consideration, the nonlocal forces at long-range between molecules and lattice lead to the nonlocal stress-strain equation with higher-order strain gradients. Because of its simplicity and superiority, the analysis of wave propagation in CNTs using the nonlocal stress approach was recently reported [Wang and Hu 2005; Wang 2005; Wang et al. 2006c; Lu et al. 2007; Heireche et al. 2008; Liew et al. 2008]. In particular, [Lu et al. 2007] derived the equation of motion for a nonlocal Timoshenko beam to investigate the wave propagation characteristics in single-walled and double-walled CNTs. Other nonlocal shell models were also employed for further research in a number of studies [Wang 2006; Wang et al. 2006b; Wang and Varadan 2007; Xie et al. 2007a; Xie et al. 2007b; Wang et al. 2008; Hu et al. 2008].

Virtually all published works [Wang and Hu 2005; Wang 2005; Wang et al. 2006c; Lu et al. 2007; Heireche et al. 2008; Liew et al. 2008; Wang 2006; Wang et al. 2006b; Wang and Varadan 2007; Xie et al. 2007a; Xie et al. 2007b; Wang et al. 2008; Hu et al. 2008] in wave propagation using the nonlocal stress approach regarded the nanoscale to only affect the constitutive relation for nonlocal stress and strain. Without rigorous validation, the classical equilibrium equations or equations of motion for beam and shell models were adopted completely for all nonlocal static and dynamic problems. Such directly extended nonlocal models, termed the partial nonlocal stress models, results in two fundamental suspicions that: (a) in many cases of study the nanoscale effect is surprisingly missing in the ultimate analytical solution, for instance the bending of a cantilever nanotube with point force at its end; and (b) the no-existence of any higher-order boundary conditions associated with the higher-order differential equation of motion

[Lim 2008; 2009; 2010]. The second statement above simply implies that the partial nonlocal stress models derives a higher-order equation of motion but, unfortunately, without the corresponding higher-order boundary conditions which is obviously inconsistent. In [Lim 2008; 2009; 2010] we successfully established a new analytical nonlocal stress model and proved that stiffness of a nanobeam is strengthened with the presence of a nonlocal nanoscale. By deriving the exact nonlocal strain energy density, higher-order governing differential equation with the corresponding higher-order boundary conditions was derived via the variational principle. New predictions for bending of nanobeams were presented and discussed.

Applying the identical nonlocal stress model but without making any assumptions on the static and dynamic conditions a priori, a new higher-order dynamics differential equation of motion are derived via exact variational principle here. Consistent higher-order boundary conditions and insightful predictions using this new model are presented. Implications of the defective formulation and intriguing conclusions in wave propagation in CNTs using the partial nonlocal stress models are also discussed in detail. The CNTs considered here are shear deformable using the thick-walled tube model in order to better reflect the nature of CNTs. Benchmarked analytical dispersion relations are derived and the contribution of nonlocal nanoscale in the governing equation of motion is highlighted. Qualitative comparisons [Nix and Gao 1998; Lam et al. 2003; Park and Hao 2006; 2008; Ma et al. 2008; Li and Chou 2004; Was and Foecke 1996; McFarland and Colton 2005] with other non-nonlocal approaches towards the end of the paper including molecular dynamics simulation, strain gradients model, couple stress model and experiments justify that the stiffness enhancement conclusion as predicted by the new nonlocal stress model.

## 2. Nonlocal elasticity stress field theory and nonlocal stress models

***Basic nonlocal constitutive equations and nonlocal stress.*** The nonlocal elastic stress field theory first proposed by Eringen concerns the state of stress at a reference point $\boldsymbol{r}'$ within a domain. The nonlocal stress depends not only on the strain at that location but also on the strains at all other points within the domain in a diminishing influence away from the central location. This phenomenon was first observed in atomic theory of lattice dynamics and also from experiment observation on phonon dispersion. In the absence of the nonlocal effects of strains at points $\boldsymbol{r} \neq \boldsymbol{r}'$, the nonlocal field theory reverts to the local or classical elasticity theory [Eringen 1983; 2002]. For homogeneous and isotropic solids with nonlocal effects, the nonlocal elastic field theory is governed by

$$\sigma_{ij,i} + \rho(f_j - \ddot{u}_j) = 0, \qquad \sigma_{ij}(\boldsymbol{r}) = \int_V \alpha(|\boldsymbol{r}' - \boldsymbol{r}|, \tau)\sigma'_{ij}(\boldsymbol{r}')\, dV(\boldsymbol{r}'), \tag{1}$$

$$\sigma'_{ij}(\boldsymbol{r}') = \lambda e_{kk}(\boldsymbol{r}')\delta_{ij} + 2\mu e_{ij}(\boldsymbol{r}'), \qquad e_{ij}(\boldsymbol{r}') = \frac{1}{2}\left(\frac{\partial u_j(\boldsymbol{r}')}{\partial \boldsymbol{r}'_i} + \frac{\partial u_i(\boldsymbol{r}')}{\partial \boldsymbol{r}'_j}\right), \tag{2}$$

where $\sigma_{ij}(\boldsymbol{r})$ is the nonlocal stress tensor, $\rho$ the mass density, $f_j$ the body force density, and $u_j$ the displacement vector at a reference point $\boldsymbol{r}$ in the body, at time $t$, while $\ddot{u}_j$, the second derivative of $u_j$ with respect to time $t$, is the acceleration vector at $\boldsymbol{r}$. The indices $i$, $j$ run over the sets $\{1\}$, $\{1, 2\}$ or $\{1, 2, 3\}$ depending on the dimension.

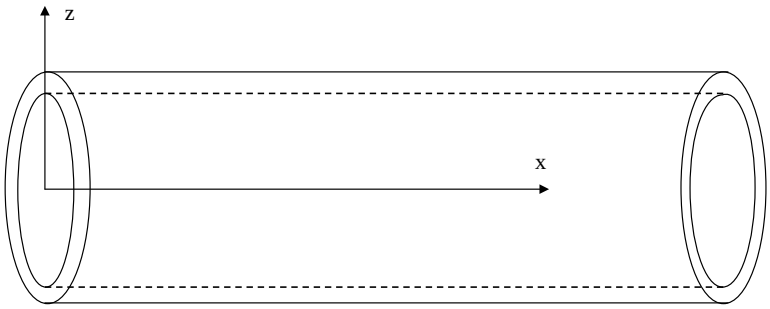


**Figure 1.** Cylindrical nanotube and coordinate system.

Equation $(2)_1$ shows the classical constitutive relation of Hooke's low where the classical or local stress tensor at $\boldsymbol{r}'$, denoted as $\sigma'_{ij}(\boldsymbol{r}')$, is related to the linear strain tensor $e_{ij}(\boldsymbol{r}')$ at any point $\boldsymbol{r}'$ in the body at time $t$, with $\lambda$ and $\mu$ being Lamé constants, and $\delta_{ij}$ being Kronecker delta. It is clear that the classical or local constitutive relation $(2)_1$ has to be replaced by the nonlocal constitutive relative $(1)_2$, according to which $\sigma_{ij}(\boldsymbol{r})$ at $\boldsymbol{r}$ depends not only on the classical local stress $\sigma'_{ij}(\boldsymbol{r}')$ at that particular point but also on a nonlocal modulus $\alpha(|\boldsymbol{r}' - \boldsymbol{r}|, \tau)$, where $|\boldsymbol{r}' - \boldsymbol{r}|$ is the Euclidean distance between $\boldsymbol{r}'$ and $\boldsymbol{r}$ and $\tau$ is a dimensionless length scale defined by

$$\tau = \frac{e_0 a}{L}, \tag{3}$$

$a$ being the internal characteristic length such that the lattice parameter, C-C bond length, or granular distance, $L$ an external characteristic length such as the crack length or wavelength, and $e_0$ is a material constant obtainable experimentally or through other molecular or continuum models.

Due to the difficulty in deriving an analytical solution, it is possible in an approximate sense to convert the integrodifferential equation $(1)_2$ to a general partial differential equation [Eringen 1983; 2002]. Furthermore, when only the uniaxial stress and strain are considered for a nanotube, the classical Hooke's law for uniaxial stress in one dimension is replaced by a nonlocal stress relation (loc. cit.) as

$$\sigma(x) - (e_0 a)^2 \frac{d^2\sigma(x)}{dx^2} = E\varepsilon(x), \tag{4}$$

where $E$ is the Young's modulus and $\sigma(x)$ and $\varepsilon(x)$ are the normal stress and strain in the axial direction of the nonlocal nanotube. For limiting nanoscale $e_0 a \to 0$, the nonlocal effect can be neglected and the nonlocal stress $\sigma$ approaches that of the corresponding classical stress $\sigma' = E\varepsilon(x)$. It is noted that (4) is a one-dimensional ordinary differential equation.

Figure 1 shows the shear deformable nanotube in Cartesian coordinate while $x$ and $z$ are the axial and transverse coordinates respectively. According to the classical elastic theory for a long tube, the bending moment $M_{xx}$ in the transverse direction and strain are denoted by

$$M_{xx} = \int z\sigma \, dA, \quad \varepsilon = -z\frac{d\varphi}{dx}, \tag{5}$$

where $z$ is the normal coordinate measured from the midplane, $\varphi(x, t)$ is the rotation angle of cross section at point $x$ and time $t$, and $A$ is the cross sectional area. Multiplying (4) by $z$, integrating over the

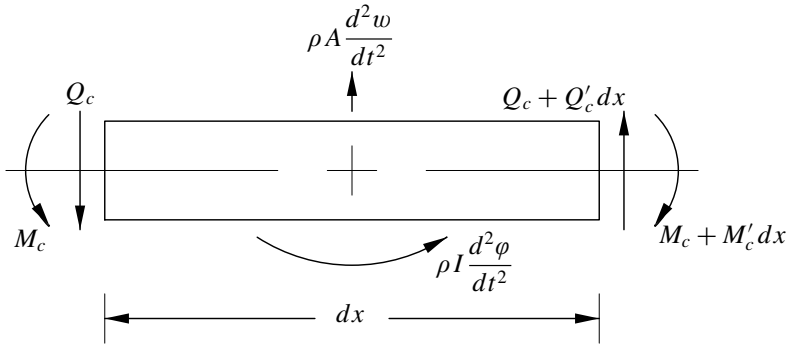


**Figure 2.** Geometry of a nanobeam, coordinate system and sign convention.

cross section and substituting Equations (5) yield the nonlocal bending moment relation as

$$M_{xx} - (e_0 a)^2 \frac{\partial^2 M_{xx}}{\partial x^2} = -EI \frac{\partial \varphi}{\partial x} \tag{6}$$

while $I = \int z^2 \, dA$ is the second moment of area over the cross section.

For simplicity and standardization, the following dimensionless terms

$$\bar{x} = \frac{x}{L}, \quad \bar{z} = \frac{z}{L} \tag{7}$$

are introduced, where $L$ can be taken as the length of the nanotube. The dimensionless solutions of (4) and (6) can be expressed as [Lim 2009; 2010]

$$\bar{\sigma}_{xx} = \sum_{n=1}^{\infty} \tau^{2(n-1)} \varepsilon_{xx}^{\langle 2(n-1) \rangle} = -\bar{z} \sum_{n=1}^{\infty} \tau^{2(n-1)} \varphi^{\langle 2n-1 \rangle}, \quad \overline{M}_{xx} = -\sum_{n=1}^{\infty} \tau^{2(n-1)} \varphi^{\langle 2n-1 \rangle}, \tag{8}$$

where $\bar{\sigma}_{xx} = \sigma_{xx}/E$, $\overline{M}_{xx} = M_{xx} L/EI$ and $\langle\ \rangle$ denotes partial differentiation with respect to $\bar{x}$. Therefore, the exact solution for the nonlocal constitutive equation of nanotube described above are expressed in infinite series in terms of strain gradients for nonlocal stress and displacement gradients for nonlocal moment in (8).

***Dynamic equations of motion.*** For a thick nanotube represented by the classical shear deformable model, the effect of shear and rotation on the nanotube cross section is significant and they should be considered. The classical dynamic governing equations of motion for transverse motion and rotational motion are respectively [Hagedorn and Dasgupta 2007]

$$\frac{dQ_c}{dx} = \rho A \frac{d^2 w}{dt^2}, \quad \frac{dM_c}{dx} - Q_c = -\rho I \frac{d^2 \varphi}{dt^2}, \tag{9}$$

where subscript '$c$' represents classical terms, $\rho$, $Q_c$, $M_c$, $w(x, t)$ are the mass density, shear force on the nanotube cross section, bending moment and deflection of the nanotube in the $z$-direction as shown in Figure 2.

The classical dimensionless expressions of (9) are

$$\frac{EI}{L^3}\frac{d\overline{Q}_c}{d\bar{x}} = \frac{\rho AL}{T^2}\frac{d^2\overline{w}}{d\bar{t}^2}, \quad \overline{Q}_c - \frac{d\overline{M}_c}{d\bar{x}} = \frac{\rho L^2}{ET^2}\frac{d^2\varphi}{d\bar{t}^2}, \tag{10}$$

where $T$ is the period of vibration, $\bar{t} = t/T$ is dimensionless time, $\overline{M}_c = M_c L/EI$ is the dimensionless classical bending moment and $\overline{Q}_c = Q_c L^2/EI$ is the dimensionless classical shear force on the cross section. In the presence of a nonlocal elastic stress field, it has been a common practice to directly replace the classical $\overline{M}_c$ in the equation of motion above and in Figure 1 with the nonlocal moment $\overline{M}_{xx}$ defined in (8) [Wang and Hu 2005; Wang 2005; Wang et al. 2006c; Lu et al. 2007; Heireche et al. 2008; Liew et al. 2008; Wang 2006; Wang et al. 2006b; Wang and Varadan 2007; Xie et al. 2007a; Xie et al. 2007b; Wang et al. 2008; Hu et al. 2008; Lim and Wang 2007]. Such models are termed the partial nonlocal models. For bending of a nanotube, it has been shown through a rigorous derivation via the variational principle that such direct replacement in the partial nonlocal derivation is not only unjustified but also results in intriguing solutions with respect to physical intuition, modeling and numerical simulation using other non-nonlocal approaches such as strain gradient, coupled stress, molecular dynamic simulation, etc., as well as experiments considering nanoscale effects. It will be verified herein that this statement can also extended to wave propagation in shear deformable carbon nanotubes.

Unlike virtually all previous analyses using nonlocal stress modeling, a true nonlocal nanotube requires that the equilibrium conditions and dynamic equations of motion should be consistently derived through consideration of a nonlocal stress field. For a thick nanotube, the correct governing equations can be derived from the virtual work variational principle by considering strain energy and kinetic energy. The strain energy density of a nanotube consists of two parts: the normal deformation strain energy density [Lim 2009; 2010]

$$u_n = u_1 + u_2 + u_3, \tag{11}$$

where

$$u_1 = \tfrac{1}{2}E\varepsilon_{xx}^2, \quad u_2 = \tfrac{1}{2}E\sum_{n=1}^{\infty}(-1)^{n+1}\tau^{2n}\big(\varepsilon_{xx}^{\langle n\rangle}\big)^2, \quad u_3 = E\sum_{n=1}^{\infty}\Big(\tau^{2(n+1)}\sum_{m=1}^{n}(-1)^{m+1}\varepsilon_{xx}^{\langle m\rangle}\varepsilon_{xx}^{\langle 2(n+1)-m\rangle}\Big), \tag{12}$$

and the shear deformation strain energy on the nanotube cross section

$$u_s = \tfrac{1}{2}G\gamma_{xz}^2, \tag{13}$$

where $G$ is the shear modulus and $\gamma_{xz}$ is the shear strain when $\gamma_{xz} = \partial\overline{w}/\partial\bar{x} - \varphi$. Details of the derivation of $u_n$ are given in the Appendix. The total strain energy of the deformed nanotube with volume $V$ is

$$U = \int_v (u_n + u_s)\, dV. \tag{14}$$

The kinetic energy $K$ of a nanotube is

$$K = \frac{\rho}{2}\int_0^L \left(A\Big(\frac{dw}{dt}\Big)^2 + I\Big(\frac{d\varphi}{dt}\Big)^2\right) dx = \frac{\rho AL^3}{2T^2}\int_0^1 \left(\Big(\frac{d\overline{w}}{d\bar{t}}\Big)^2 + \frac{I}{AL^2}\Big(\frac{d\varphi}{d\bar{t}}\Big)^2\right) d\bar{x}. \tag{15}$$

The first term in the integral contributes to the translational kinetic energy while the second term contributes to the rotational kinetic energy. Define the total energy functional $F$ as

$$F = U - K. \tag{16}$$

Substituting Equations (11)–(15) into (16) yields the variation of the energy functional $F$ as

$$\begin{aligned}
\delta F &= \delta(U-K) \\
&= \delta \int_0^1 \int_V \Bigg( \tfrac{1}{2} E \varepsilon_x^2 + \tfrac{1}{2} E \sum_{n=1}^{\infty} (-1)^{n+1} \tau^{2n} \big(\varepsilon_x^{\langle n \rangle}\big)^2 \\
&\qquad + E \sum_{n=1}^{\infty} \Big( \tau^{2(n+1)} \sum_{m=1}^{n} (-1)^{m+1} \varepsilon_x^{\langle m \rangle} \varepsilon_x^{\langle 2(n+1)-m \rangle} \Big) + \tfrac{1}{2} G \gamma_{xz}^2 \Bigg) dV \, d\bar{t} \\
&\qquad\qquad - \delta \frac{\rho A L^3}{2T^2} \int_0^1 \int_0^1 \left( \left( \frac{\partial \overline{w}}{\partial \bar{t}} \right)^2 + \frac{I}{AL^2} \left( \frac{\partial \varphi}{\partial \bar{t}} \right)^2 \right) d\bar{x} \, d\bar{t} \\
&= \delta \int_0^1 \int_V \Bigg( -\tfrac{1}{2} E z \left( \frac{\partial \varphi}{\partial \bar{x}} \right)^2 - \tfrac{1}{2} E z \sum_{n=1}^{\infty} (-1)^{n+1} \tau^{2n} \big(\varphi^{\langle n+1 \rangle}\big)^2 \\
&\qquad + E z^2 \sum_{n=1}^{\infty} \Big( \tau^{2(n+1)} \sum_{m=1}^{n} (-1)^{m+1} \varphi^{\langle m+1 \rangle} \varphi^{\langle 2n-m+1 \rangle} \Big) + \tfrac{1}{2} G \left( \frac{\partial \overline{w}}{\partial \bar{x}} - \varphi \right)^2 \Bigg) dV \, d\bar{t} \\
&\qquad\qquad - \delta \frac{\rho A L^3}{2T^2} \int_0^1 \int_0^1 \left( \left( \frac{\partial \overline{w}}{\partial \bar{t}} \right)^2 + \frac{I}{AL^2} \left( \frac{\partial \varphi}{\partial \bar{t}} \right)^2 \right) d\bar{x} \, d\bar{t} \\
&= \int_0^1 \int_V \Bigg( -E z \varphi^{\langle 1 \rangle} \, \delta\varphi^{\langle 1 \rangle} - E z \sum_{n=1}^{\infty} (-1)^{n+1} \tau^{2n} \varphi^{\langle n+1 \rangle} \, \delta\varphi^{\langle n+1 \rangle} \\
&\qquad + E z^2 \sum_{n=1}^{\infty} \Big( \tau^{2(n+1)} \sum_{m=1}^{n} (-1)^{m+1} \big( \delta\varphi^{\langle m+1 \rangle} \varphi^{\langle 2n-m+1 \rangle} + \varphi^{\langle m+1 \rangle} \, \delta\varphi^{\langle 2n-m+1 \rangle} \big) \Big) \\
&\qquad\qquad + \tfrac{1}{2} G \big( 2\overline{w}^{\langle 1 \rangle} \, \delta\overline{w}^{\langle 1 \rangle} - 2\overline{w}^{\langle 1 \rangle} \, \delta\varphi - 2\varphi \, \delta\overline{w}^{\langle 1 \rangle} + 2\varphi \, \delta\varphi \big) \Bigg) dV \, d\bar{t} \\
&\qquad\qquad\qquad - \frac{\rho A L^3}{2T^2} \int_0^1 \int_0^1 \left( 2\ddot{\overline{w}} \, \delta\ddot{\overline{w}} + \frac{2I}{AL^2} \ddot{\varphi} \, \delta\ddot{\varphi} \right) d\bar{x} \, d\bar{t}.
\end{aligned} \tag{17}$$

Integrating (17) by parts for each term in the integrand, we obtain

$$\begin{aligned}
\delta F = {} & \frac{EI}{L} \int_0^1 \int_0^1 \left( \frac{AG\kappa L^2}{EI} \left( \frac{\partial \overline{w}}{\partial \bar{x}} - \varphi \right) - \sum_{n=1}^{\infty} (2n-3) \tau^{2(n-1)} \varphi^{\langle 2n \rangle} - \frac{\rho L^2}{ET^2} \frac{\partial^2 \varphi}{\partial \bar{t}^2} \right) \delta\varphi \, d\bar{x} \, d\bar{t} \\
& + \int_0^1 \int_0^1 \left( AG\kappa L \left( \frac{\partial^2 \overline{w}}{\partial \bar{x}^2} - \frac{\partial \varphi}{\partial \bar{x}} \right) - \frac{\rho A L^3}{T^2} \frac{\partial^2 \overline{w}}{\partial \bar{t}^2} \right) \delta\overline{w} \, d\bar{x} \, d\bar{t} \\
& + \frac{EI}{L} [\varphi \, \delta\varphi]_0^1 + \frac{EI}{L} \sum_{n=1}^{\infty} \left( (-1)^{n+1} \tau^{2n} \sum_{m=0}^{n+1} \varphi^{\langle n+1+m \rangle} \, \delta\varphi^{\langle n-m \rangle} \Big|_0^1 \right) \\
& + \frac{EI}{L} \sum_{n=1}^{\infty} \tau^{2(n+1)} \sum_{m=1}^{n} \Bigg( \sum_{i=0}^{2n+1-m} (-1)^{m+i+1} \varphi^{\langle 2+m+i \rangle} \, \delta\varphi^{\langle 2n+1-m-i \rangle} \Big|_0^1 \\
& \qquad + \sum_{i=0}^{m-1} (-1)^{m+i+1} \varphi^{\langle 2n+2-m+i \rangle} \, \delta\varphi^{\langle 1+m-i \rangle} \Big|_0^1 \Bigg),
\end{aligned} \tag{18}$$

Using the definition of nonlocal bending moment in $(8)_2$, the variation of the energy functional in (18) can be rewritten as

$$\begin{aligned}\delta F = \int_0^1 \int_0^1 \Bigg( \frac{EI}{L}\Big(\overline{Q} - \overline{M}_{xx}^{\langle 1\rangle} + 2\sum_{n=1}^{\infty} \tau^{2n} \overline{M}_{xx}^{\langle 2n+1\rangle} - \frac{\rho L^2}{ET^2}\frac{\partial^2 \varphi}{\partial \bar{t}^2}\Big)\delta\varphi + \Big(\frac{EI}{L}\frac{\partial \overline{Q}}{\partial \bar{x}} - \frac{\rho AL^3}{T^2}\frac{\partial^2 \overline{w}}{\partial \bar{t}^2}\Big)\delta\overline{w}\Bigg)\, d\bar{x}\, d\bar{t} \\ + \frac{EI}{L}\Bigg[\Big(\overline{Q} - \overline{M}_{xx}^{\langle 1\rangle} - 2\sum_{n=1}^{\infty} \tau^{2n} \overline{M}_{xx}^{\langle 2n+1\rangle}\Big)\delta\varphi + \Big(-\overline{M}_{xx} + 2\sum_{n=1}^{\infty} \tau^{2n} \overline{M}_{xx}^{\langle 2n\rangle}\Big)\delta\varphi^{\langle 1\rangle} \\ - \Big(\tau^2 \overline{M}_{xx}^{\langle 1\rangle} + 2\sum_{n=1}^{\infty} \tau^{2(n+1)} \overline{M}_{xx}^{\langle 2n+1\rangle}\Big)\delta\varphi^{\langle 2\rangle} + \Big(2\tau^4 \sum_{n=1}^{\infty} \tau^{2(n-1)} \overline{M}_{xx}^{\langle 2n\rangle}\Big)\delta\varphi^{\langle 3\rangle} \\ - \Big(\tau^4 \overline{M}_{xx}^{\langle 1\rangle} + 2\sum_{n=1}^{\infty} \tau^{2(n+2)} \overline{M}_{xx}^{\langle 2n+1\rangle}\Big)\delta\varphi^{\langle 4\rangle} + \Big(\tau^6 \overline{M}_{xx}^{\langle 2\rangle} + 2\sum_{n=1}^{\infty} \tau^{2(n+3)} \overline{M}_{xx}^{\langle 2(n+1)\rangle}\Big)\delta\varphi^{\langle 5\rangle} \cdots \Bigg]_0^1, \end{aligned} \tag{19}$$

where

$$\overline{Q} = \frac{AG\kappa L^2}{EI}\Big(\frac{\partial \overline{w}}{\partial \bar{x}} - \varphi\Big) \tag{20}$$

is the dimensionless form of the shear force $Q = \int_A G\gamma_{xz}\, dA = AG\kappa(\partial w/\partial x - \varphi)$ on the cross section of the nanotube [Hagedorn and Dasgupta 2007], and $\kappa$ is the shear correction factor due to shear deformation in nanotube.

The variational principle requires the variation of energy function to be zero at an extremum:

$$\delta F = \delta(U - K) = 0. \tag{21}$$

Because $\overline{w}$, $\varphi$, $\varphi^{\langle 1\rangle}$, $\varphi^{\langle 2\rangle}$, $\varphi^{\langle 3\rangle}$, ... are arbitrary functions whose variations do not vanish, the variational principle requires that their multipliers be zero. From the first two terms in the integrand in (19), the governing equations of motion for a shear deformable nanotube are

$$\frac{EI}{L}\frac{\partial \overline{Q}}{\partial \bar{x}} = \frac{\rho AL^3}{T^2}\frac{\partial^2 \overline{w}}{\partial \bar{t}^2}, \quad \overline{Q} - \frac{\partial \overline{M}_{xx}}{\partial \bar{x}} + 2\sum_{n=1}^{\infty} (\tau)^{2n} \frac{\partial^{(2n+1)} \overline{M}_{xx}}{\partial \bar{x}^{(2n+1)}} = \frac{\rho L^2}{ET^2}\frac{\partial^2 \varphi}{\partial \bar{t}^2} \tag{22}$$

the second of which can be rewritten as

$$\overline{Q} - \frac{\partial \overline{M}_{\mathrm{ef}}}{\partial \bar{x}} = \frac{\rho L^2}{ET^2}\frac{\partial^2 \varphi}{\partial \bar{t}^2}, \tag{23}$$

where

$$\overline{M}_{\mathrm{ef}} = \overline{M}_{xx} - 2\sum_{n=1}^{\infty} \tau^{2n} \overline{M}_{xx}^{\langle 2n\rangle} = \sum_{n=1}^{\infty} (2n-3)\tau^{2(n-1)} \varphi^{\langle 2n-1\rangle} \tag{24}$$

is defined as the effective dimensionless nonlocal moment $\overline{M}_{\mathrm{ef}}$. The remaining terms in (19) constitute the higher-order boundary conditions which have been unavailable in all other research papers of nonlocal wave propagation [Wang and Hu 2005; Wang 2005; 2006; Wang et al. 2006b; 2006c; 2008; Lu et al. 2007; Heireche et al. 2008; Liew et al. 2008; Wang and Varadan 2007; Xie et al. 2007a; 2007b; Hu et al. 2008]. These equations of motion and the corresponding higher-order boundary conditions are new and their physical interpretation and consequence will be discussed at length in due course.

Equations (22) and (23) represent the transverse equation of motion and rotational equation of motion, respectively, and they are expressed in terms of nonlocal stress resultants. These two equations can also be expressed in terms of dimensionless deflection $\overline{w}$ and angle of rotation $\varphi$ as

$$G\kappa L\left(\frac{\partial^2\overline{w}}{\partial\bar{x}^2}-\frac{\partial\varphi}{\partial\bar{x}}\right)-\frac{\rho L^3}{T^2}\frac{\partial^2\overline{w}}{\partial\bar{t}^2}=0, \tag{25}$$

$$\frac{AG\kappa L^2}{EI}\left(\frac{\partial\overline{w}}{\partial\bar{x}}-\varphi\right)-\sum_{n=1}^{\infty}(2n-3)\tau^{2(n-1)}\varphi^{\langle 2n\rangle}-\frac{\rho L^2}{ET^2}\frac{\partial^2\varphi}{\partial\bar{t}^2}=0. \tag{26}$$

Equations (25) and (26) are obtained from the first two terms in the integration in (18). Alternatively, (25) and (26) can be obtained by substituting $(8)_2$ and (20) into (23) and (24).

***Wave propagation in a shear deformable carbon nanotube.*** For analyzing the effect of $\tau$ on wave propagation in a carbon nanotube, terms of order $O(\tau^6)$ in the equations of motion are omitted. The corresponding expressions for (25) and (26) are

$$G\kappa L\left(\frac{\partial^2\overline{w}}{\partial\bar{x}^2}-\frac{\partial\varphi}{\partial\bar{x}}\right)=\frac{\rho L^3}{T^2}\frac{\partial^2\overline{w}}{\partial\bar{t}^2}, \tag{27}$$

$$\frac{AG\kappa L^2}{EI}\left(\frac{\partial\overline{w}}{\partial\bar{x}}-\varphi\right)+\frac{\partial^2\varphi}{\partial\bar{x}^2}-\tau^2\frac{\partial^4\varphi}{\partial\bar{x}^4}-3\tau^4\frac{\partial^6\varphi}{\partial\bar{x}^6}=\frac{\rho L^2}{ET^2}\frac{\partial^2\varphi}{\partial\bar{t}^2}. \tag{28}$$

For wave propagation, the functions of deflection $\overline{w}(\bar{x},\bar{t})$ and rotation $\varphi(\bar{x},\bar{t})$ are expressed as

$$\overline{w}(x,t)=\overline{W}e^{i(\bar{k}\bar{x}-\bar{\omega}\bar{t})}, \tag{29}$$

$$\varphi(x,t)=\Phi e^{i(\bar{k}\bar{x}-\bar{\omega}\bar{t})}, \tag{30}$$

where $k$ is wavenumber, $\omega$ is angle frequency and the dimensionless forms of these two variables are $\bar{k}=kL$ and $\bar{\omega}=\omega T$. Hence (27) and (28) can be reduced to linear system

$$\left(\frac{\rho L^3}{T^2}\bar{\omega}^2-\frac{G\kappa}{L}\bar{k}^2\right)\overline{W}-i\frac{G\kappa}{L}\bar{k}\Phi=0, \tag{31}$$

$$i\frac{AG\kappa L^2}{EI}\bar{k}^3\overline{W}+\left(\frac{\rho L^2}{ET^2}\bar{\omega}^2-\frac{AG\kappa L^2}{EI}-k^2-\tau^2\bar{k}^4+3\tau^4\bar{k}^6\right)\Phi=0, \tag{32}$$

or, in matrix form, as

$$\boldsymbol{A}\boldsymbol{x}=0, \tag{33}$$

where the elements of the matrix $\boldsymbol{A}$ are

$$\begin{aligned}
a_{11}&=\frac{\rho L^3}{T^2}\bar{\omega}^2-\frac{G\kappa}{L}\bar{k}^2,\quad a_{12}=-i\frac{G\kappa}{L}\bar{k},\quad a_{21}=i\frac{AG\kappa L^2}{EI}\bar{k}^3,\\
a_{22}&=\frac{\rho L^2}{ET^2}\bar{\omega}^2-\frac{AG\kappa L^2}{EI}-k^2-\tau^2\bar{k}^4+3\tau^4\bar{k}^6,
\end{aligned} \tag{34}$$

and the vector of generalized displacements is

$$\boldsymbol{x}=\left\{\overline{W}\ \ \Phi\right\}^T. \tag{35}$$

For nontrivial solutions of $\overline{W}$ and $\Phi$ in (33), we must have $|\boldsymbol{A}| = 0$ in (34), which yields the characteristic equation

$$\frac{\rho^2 L^5}{ET^4}\bar{\omega}^4 - \frac{GL\kappa\rho}{ET^2}\left(\bar{k}^2 + \frac{AL^4}{I}\right)\bar{\omega}^2 + \left(\frac{G\kappa}{L} - \frac{\rho L^3}{T^2}\right)(1 + \tau^2\bar{k}^2 - 3\tau^4\bar{k}^4)\bar{k}^2 = 0. \tag{36}$$

This is a quartic equation whose roots are

$$\bar{\omega}_{1,2,3,4} = \pm\sqrt{\frac{-b_1 \pm \sqrt{b_1^2 - 4a_1c_1}}{2a_1}}, \tag{37}$$

where $a_1$, $b_1$ and $c_1$ are defined in terms of $\bar{k}$ as

$$a_1 = \frac{\rho^2 L^5}{ET^4}, \quad b_1 = -\frac{GL\kappa\rho}{ET^2}\left(\bar{k}^2 + \frac{AL^4}{I}\right), \quad c_1 = \left(\frac{G\kappa}{L} - \frac{\rho L^3}{T^2}\right)(1 + \tau^2\bar{k}^2 - 3\tau^4\bar{k}^4)\bar{k}^2. \tag{38}$$

Equations (37) and (38) give the spectrum relation between $\omega$ and $k$ based on this new analytical nonlocal shear deformable nanotube model. Using the partial nonlocal nanotube model, the corresponding relation is identical to (37) except that $a_1$, $b_1$, $c_1$ be replaced by $a_2$, $b_2$, $c_2$, given by [Liew et al. 2008]

$$a_2 = \frac{\rho^2 L^5}{ET^4}, \quad b_2 = -\frac{GL\kappa\rho}{ET^2}\left(\bar{k}^2 + \frac{AL^4}{I}\right), \quad c_2 = \left(\frac{G\kappa}{L} - \frac{\rho L^3}{T^2}\right)(1 - \tau^2\bar{k}^2 + \tau^4\bar{k}^4)\bar{k}^2. \tag{39}$$

Obviously the only difference between the solutions of this new analytical nonlocal stress model and the existing partial nonlocal stress model [Liew et al. 2008] is contributed by $c_1$ and $c_2$. The difference leads to different characteristics of the two dispersion relations and spectrum relations for wave propagation in CNTs as discussed in great details in the following section.

## 3. Results and discussion

***Effects of nanoscale on dispersion relation.*** We now present some numerical examples to illustrate the contrast between the analytical nonlocal shear deformable nanotube model (ANT) and the partial nonlocal shear deformable nanotube model (PNT) for wave propagation in a nonlocal nanotube with respect to the classical shear deformable tube model (CT). In these examples, the nanotubes are considered as homogeneous and isotropic with geometric and materials properties as in [Liew et al. 2008]: diameter $d = 5\,\text{nm}$, thickness $t = 0.34\,\text{nm}$, length $L = 10\,\text{nm}$, Young's modulus $E = 0.72\,\text{TPa}$, Poisson's ratio $\upsilon = 0.254$, density $\rho = 2.3\,\text{g/cm}^3$, vibration period $T = 4 \times 10^{-13}\,\text{s}$ and shear correction factor $\kappa = \frac{10}{9}$.

The dispersion relation between the dimensionless phase velocity $\bar{c}$ and the dimensionless wave number $\bar{k}$ (where $\bar{c} = \bar{\omega}/\bar{k}$) with various $\tau$ is illustrated in Figure 3 for shear deformable nanotube models based on the PNT solution in (37) and (39) and the ANT solution in (37) and (38). The classical wave propagation solution for the classical shear deformable nanotube without nonlocal effects can be deduced by substituting $\tau = 0$ in (38) or (39).

The different dispersion relations based on ANT, PNT and CT are indicated in Figure 3. For the dispersion relation based on the CT model, the phase velocity increases linearly for $\bar{k} < 15$ approximately, while a constant $\bar{c}$ is observed at higher wavenumbers. For PNT models, there exists a critical wavenumber $\bar{k}_{\text{cri}}$ below which the dispersion relation is close to linear and similar to the classical CT solution. Past $\bar{k}_{\text{cri}}$, linearity fails, and eventually the velocity starts dropping as the wavenumber becomes sufficiently

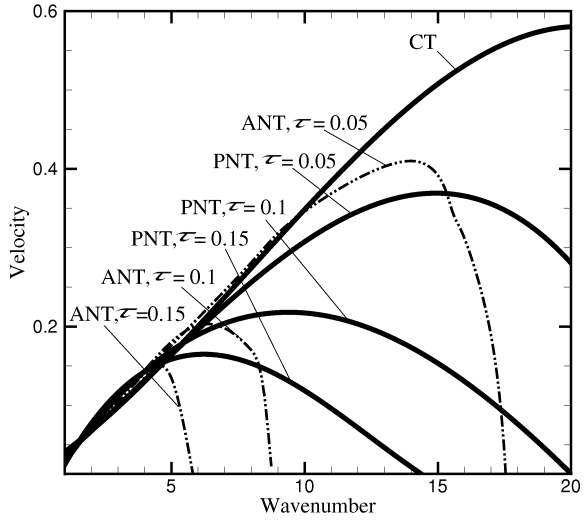


**Figure 3.** Dispersion relation obtained from shear deformable nanotube model.

high. For ANT models, there is also a critical wavenumber below which the phase velocity exceeds the PNT and CT values. For instance, for $\bar{k} = 5$ and $\tau = 0.1$, the phase velocity is $\bar{c} = 0.18$ according to ANT, $\bar{c} = 0.17$ for CT and $\bar{c} = 0.16$ for PNT. In other words, nonlocality in nanotubes has a stiffening effect (increase in phase velocity) according to ANT, relative to the classical solutions, but the opposite effect according to PNT. Past the critical wavenumber, the ANT-predicted phase velocity drops sharply, differing significantly from the of CT and PNT solutions. Thus, according to ANT, wave propagation in shear deformable nanotubes decay rapidly after the wavenumber exceeds critical value.

Figure 4 plots the dimensionless angle frequency $\bar{\omega}$ versus the wavenumber $\bar{k}$ for various $\tau$ based on the different nanotube models. For the classical model, the predicted frequency keeps increasing with

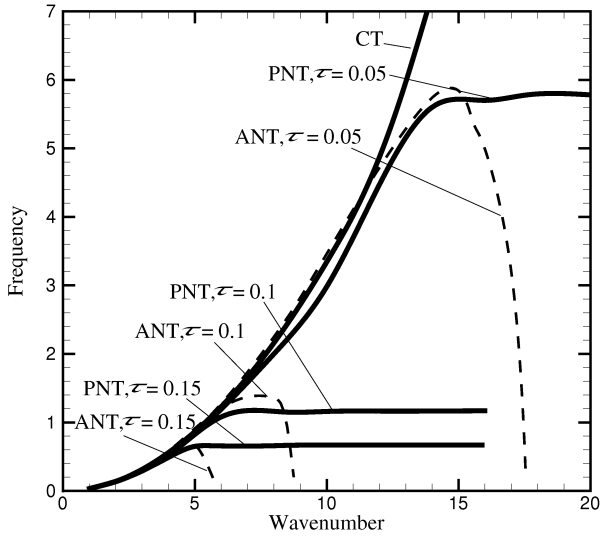


**Figure 4.** Spectrum relation obtained from shear deformable nanotube model.

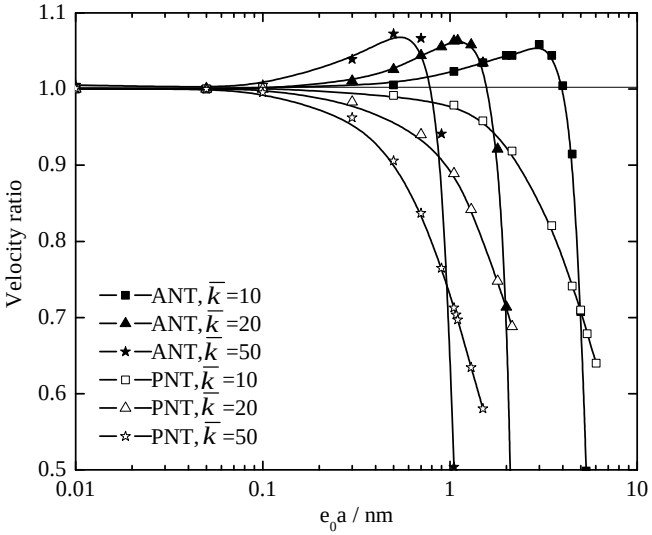


**Figure 5.** Effect of scale parameter ($\tau$) on the ratio of the phase velocity predicted by our models (ANT and PNT) to the classical (CT) solution, for the shear deformable nanotube model.

the wavenumber. For PNT, it flattens out for wavenumbers beyond the critical value $\bar{k}_{\text{cri}}$. For ANT, the frequency at first increases as in the first two models but then drops sharply.

As we saw in connection with Figure 3, ANT predicts stiffening below the critical wavenumber, while the opposite is predicted by PNT. This can also be observed in the frequency/wavenumber relation: for $\bar{k} = 4$ and $\tau = 0.1$, the predicted frequency is $\bar{\omega} = 0.8$ according to ANT, $\bar{\omega} = 0.7$ according to PNT, and $\bar{\omega} = 0.75$ according to CT.

The presence of a frequency maximum under ANT and the subsequent decay are mainly due to the strong nanoscale effect contributed by the nonlocal (long-range) stress between molecules and lattice at high wavenumbers. The critical wavenumber decreases from 14 to 5 as the nanoscale parameter $\tau$ increases from 0.05 to 0.15. It implies for stronger nanoscale effect, the decay wave propagation in nanotube is more ready to be induced at lower a wavenumber.

The influence of a small scale effect on the dispersion relations is further illustrated in Figure 5, which plots the velocity ratio relative to the classical solution as a function of $\tau$, for different values of $\bar{k}$. We see in this figure that the phase velocity according to the ANT and PNT nonlocal models are very close to the classical solutions for $\tau < 0.03$; thus wave propagation in the nanotube is hardly influenced by nanoscale effects in this range. A sharp reduction in wave propagation velocity then occurs for larger $\tau$. A critical point $\tau_{\text{cri}}$ is seen on each ANT and PNT, which decreases as the wave number increases. Thus, ANT predicts the values 0.6, 1.2, and 2 for $\tau_{\text{cri}}$ when $\bar{k} = 50$, 20, and 10, respectively. This is consistent with the expectation that propagation at a higher wavenumber requires more kinetic energy. The contribution due to the presence nanoscale $\tau$ is decreasingly sufficient to sustain such status of wave propagation and hence a smaller $\tau_{\text{cri}}$ corresponds to a higher wavenumber.

As stated in (3), $\tau$ is dimensionless quantity representing the small scale parameter $e_0 a$. According to Eringen's theory of nonlocal elasticity [Eringen and Edelen 1972; Eringen 1972a; 1972b; 1983; 2002], the internal characteristic length $a$ of material is a simple lattice parameter such as the granular distance

or bond length. For CNTs, this value could be considered as the C-C bond length, or $a = 0.142\,\text{nm}$ on average [Wang 2005; 2006; Wang et al. 2006b; 2006c; 2008; Lu et al. 2007; Heireche et al. 2008; Liew et al. 2008; Wang and Varadan 2007; Xie et al. 2007a; 2007b; Hu et al. 2008]. The material constant $e_0$ is a parameter that indicates the small scale effect on the material properties [Eringen 2002] and it was stated as $e_0 = 0.39$ in [Eringen 1983; 2002]. This result should be further confirmed by experiment or other approaches such as MD or matching the dispersion relation of atomic lattice dynamics. Furthermore, the value of $e_0$ is not a constant for different materials and small scale nanostructures. For research of wave propagation in CNTs, the value of $e_0$ could possibly be in the range $0 < e_0 a < 210\,\text{nm}$ [Wang 2005]. In this paper, $0 \le \tau \le 5$ is assumed for comparison between ANT and PNT. For a specific CNT with $L = 10\,\text{nm}$, this implies $0 < e_0 a < 50\,\text{nm}$. As shown in Figure 5, wave propagation decays very fast when $\tau > \tau_{\text{cri}}$, which means $e_0 a$ could not be too high and its specific range depends on $L$.

It is also clear from Figure 5 that the phase velocity ratios of PNT are never beyond unity while the corresponding ANT solutions are different for small $\tau$ below the critical value. Thus stiffness enhancement of nanotube by the presence of nanoscale effect via ANT is further confirmed in this example.

***Comparison with molecular dynamic simulation.*** The MD approach is considered as an authoritative means to analyze CNTs and extensive research based on MD simulation on the mechanics properties of CNTs has been published [Liew et al. 2004a; 2004b; 2005; 2008; Kitipornchai et al. 2005; Wang and Hu 2005; Wang et al. 2006b; 2008; Hu et al. 2008]. Other approaches or models are often compared with MD to verify the solutions. For this reason and to further confirm the validity of the ANT solutions, we present in Figure 6 a comparison of the various dispersion relations with MD results [Liew et al. 2008] for a (5, 5) CNT. In this example, the parameters and properties of nanotube are the same as in the previous subsection, except that we take the Young's modulus to be $E = 0.897\,\text{TPa}$, the diameter $d = 0.96\,\text{nm}$ and $\tau = 0.00355$.

As shown in Figure 6, all solutions seem to agree well for $\bar{k} < 1$ with respect to the classical solutions. Consistent with the previous example, the MD simulation also predicts the presence of a critical wave

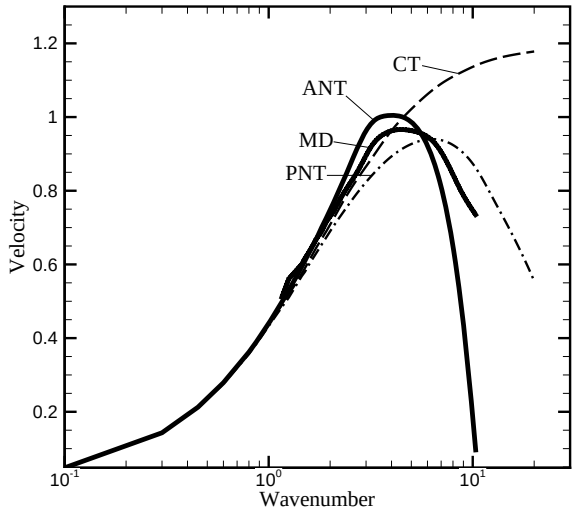


**Figure 6.** Dispersion relation obtained from different models.

velocity for sufficiently high wavenumber. In this case, wave velocity decreases for $\bar{k} > \bar{k}_{\text{cri}}$. In addition, the ANT and MD solutions both predict $\bar{k}_{\text{cri}} \approx 4$ and they agree more as compared to PNT which predicts $\bar{k}_{\text{cri}} \approx 6$. The classical model fails to predict the existence of any critical wavenumber at all.

The comparison should be interpreted in the following manner. The classical solutions without nanoscale effects should be viewed as the demarcation between the various models. As the wavenumber increases (smaller wavelength) which indicates more prominent nanoscale influence, on one side of the demarcation shows increasing wave velocity or equivalently higher stiffness (wave propagates faster in a more stiff medium) while on the other side of the demarcation shows decreasing wave velocity and hence decreasing stiffness. It is clear that the analytical nonlocal stress and MD approaches both predict comparable solutions while the partial nonlocal stress model predicts otherwise. This comparison with MD solutions concludes that the analytical nonlocal stress model is consistent with MD solutions. It should be noted that for very high wavenumber, the curves do not agree well. At such length scales which attain sub-nano ranges, one full wavelength only covers a limited number of molecules and the medium may not be continuous. In such sub-nano ranges, the validity of all continuum CNT models has to be further investigated.

In conclusion, it is confirmed that the ANT model predicts more agreeable solutions with respect to MD simulations in terms of critical values as well stiffness and wave velocity enhancement as compared to PNT.

## 4. Further discussion on the analytical nonlocal and partial nonlocal modeling

Equations (22) and (23) express the governing equations of motion for a shear deformable nanotube which is derived from the variational principle. Comparing with the classical tube dynamic conditions in (9), consequently, it is concluded that the transverse equation of motion is identical for both the classical model and the nonlocal stress model, or

$$Q_c = Q \tag{40}$$

while for the bending moment equation of motion, the classical bending moment $\overline{M}_c$ should be replaced by the effective nonlocal bending moment $\overline{M}_{\text{ef}}$ defined in (24) for a nanotube with nonlocal effects.

In virtually all published works in wave propagation based on the partial nonlocal stress model [Wang and Hu 2005; Wang 2005; Wang et al. 2006c; Lu et al. 2007; Heireche et al. 2008; Liew et al. 2008; Wang 2006; Wang et al. 2006b; Wang and Varadan 2007; Xie et al. 2007a; Xie et al. 2007b; Wang et al. 2008; Hu et al. 2008], the dynamic equations of motion were derived by directly replacing the classical bending moment condition in $(9)_2$ with the nonlocal bending moment defined in (6). The direct replacement yields

$$\overline{Q} - \frac{\partial \overline{M}_{xx}}{\partial \bar{x}} = \frac{\rho L^2}{ET^2} \frac{\partial^2 \varphi}{\partial \bar{t}^2} \tag{41}$$

which was not consistent with the variational principle. By retaining terms of $O(\tau^4)$ in (23) in order to analyze the effect of nanoscale $\tau$, a truncated dynamic equation is obtained as expressed in (28). Similarly, by substituting the expression $(8)_2$ for the nonlocal moment $\overline{M}_{xx}$ in into (40) and retaining terms of $O(\tau^4)$, we obtain

$$\frac{AG\kappa L^2}{EI}\left(\frac{\partial \overline{w}}{\partial \bar{x}} - \varphi\right) + \frac{\partial^2 \varphi}{\partial \bar{x}^2} + \tau^2 \frac{\partial^4 \varphi}{\partial \bar{x}^4} + \tau^4 \frac{\partial^6 \varphi}{\partial \bar{x}^6} = \frac{\rho L^2}{ET^2} \frac{\partial^2 \varphi}{\partial \bar{t}^2}. \tag{42}$$

Comparing (23) and (40), or equivalently comparing (28) and (42) for terms $O(\tau^4)$, it is concluded that the partial nonlocal stress model predicts different nonlocal responses for bending and wave propagation as what have been illustrated in the previous examples.

Equations (22) and (23) in terms of nonlocal stress resultants, or (25) and (26) in terms of displacement and rotation, are novel governing dynamic equations of motion for a nanotube with nonlocal effect derived using an exact variational principle. These two equations govern the exact dynamic motion for a nonlocal shear deformable nanotube. These are new equations of motion first derived here and they are fundamentally distinct with respect to virtually all previous works. Verification and application of this new analytical model for analyzing the wave propagation in nanotubes have been demonstrated in the previous sections.

The conclusion of stiffness strengthening effect of nanotubes with increasing nanoscale effect is consistent qualitatively with other published research works via other non-nonlocal elasticity approaches. Some noted instances including the strain gradient theory [Nix and Gao 1998; Lam et al. 2003]; a modified couple stress theory at microscale [Park and Hao 2006; 2008, Ma et al. 2008]; computational atomistic modeling for free vibration of a carbon nanotube [Li and Chou 2004] which concluded that the fundamental frequencies of the classical solution could be significantly lower than the atomistic simulation solutions by 40% to 60%; as well as experimental studies on monolithic films [Was and Foecke 1996], on harness of nanoindentation of crystalline materials [Nix and Gao 1998], on significant increased bending stiffness of a nano-cantilever [Lam et al. 2003; McFarland and Colton 2005]. It is noted that some of the analyses above [Park and Hao 2006; 2008, Ma et al. 2008] considered only effects at microscale instead of nanoscale. It is not a concern here as to whether it is still valid at nanoscale. In this paper, the formulations are all non-dimensionalized and hence the presence of a small-scale $\tau$ indicates the deviation expected from the classical theory when size effect is present, irrespective of the actual size of $\tau$. The paper concludes that the presence of $\tau$ induces a minute structure with higher stiffness and the conclusion is consistent with the prediction of the modified couple stress theory [Park and Hao 2006; 2008, Ma et al. 2008].

## 5. Conclusions

An analytical nonlocal stress model for wave propagation in CNTs has been established through consistent variational principle. The CNTs are simulated as shear deformable nanotubes with size dependent nonlocal effects. New dynamic equations of motion for wave propagation in CNTs have been derived and new wave propagation behaviors that nonlocal stress enhances stiffness and wave velocity in CNTs have been predicted.

Analytical expressions for the dispersion relation which relates wavenumber and phase velocity and the spectrum relation (frequency versus wavenumber) are presented through the analytical nonlocal stress approach. It has been shown that there exist critical points for the dispersion relation and spectrum relation by the analytical nonlocal models and these points depend on the nanoscale parameter. For wavenumber beyond these critical values, wave propagation is decreased sharply. Furthermore, the analytical nonlocal model confirms that the nanoscale effect promotes wave propagation in nanotube for wavenumber below the critical points. The phenomenon is verified by comparison with molecular dynamic simulation.

## Appendix

The strain energy density of a nanotube due to normal deformation $u_n$ as presented in (10) and (11) [Lim 2009; 2010] can be derived as follows. From $(8)_1$, $u_n$ can be expressed as

$$u_n = \int_0^{\varepsilon_{xx}} \sigma_{xx}\, d\varepsilon_{xx} = E \sum_{n=1}^{\infty} \tau^{2(n-1)} \int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 2(n-1)\rangle}\, d\varepsilon_{xx}.$$

Since we have

$$\begin{aligned}
&\int_0^{\varepsilon_{xx}} \varepsilon_{xx} d\varepsilon_{xx} = \tfrac{1}{2}\varepsilon_{xx}^2,\\
&\int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 2\rangle} d\varepsilon_{xx} = \int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 1\rangle} d\varepsilon_{xx}^{\langle 1\rangle} = \tfrac{1}{2}(\varepsilon_{xx}^{\langle 1\rangle})^2,\\
&\int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 4\rangle} d\varepsilon_{xx} = \int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 1\rangle} d\varepsilon_{xx}^{\langle 3\rangle} = \varepsilon_{xx}^{\langle 1\rangle}\varepsilon_{xx}^{\langle 3\rangle}|_0^{\varepsilon_{xx}} - \int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 3\rangle} d\varepsilon_{xx}^{\langle 1\rangle} = \varepsilon_{xx}^{\langle 1\rangle}\varepsilon_{xx}^{\langle 3\rangle} - \int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 2\rangle} d\varepsilon_{xx}^{\langle 2\rangle}\\
&\qquad = \varepsilon_{xx}^{\langle 1\rangle}\varepsilon_{xx}^{\langle 3\rangle} - \tfrac{1}{2}(\varepsilon_{xx}^{\langle 2\rangle})^2,\\
&\int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 6\rangle} d\varepsilon_{xx} = \int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 1\rangle} d\varepsilon_{xx}^{\langle 5\rangle} = \varepsilon_{xx}^{\langle 1\rangle}\varepsilon_{xx}^{\langle 5\rangle}|_0^{\varepsilon_{xx}} - \int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 5\rangle} d\varepsilon_{xx}^{\langle 1\rangle} = \varepsilon_{xx}^{\langle 1\rangle}\varepsilon_{xx}^{\langle 5\rangle} - \int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 4\rangle} d\varepsilon_{xx}^{\langle 2\rangle}\\
&\qquad = \varepsilon_{xx}^{\langle 1\rangle}\varepsilon_{xx}^{\langle 5\rangle} - \varepsilon_{xx}^{\langle 2\rangle}\varepsilon_{xx}^{\langle 4\rangle}|_0^{\varepsilon_{xx}} + \int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 4\rangle} d\varepsilon_{xx}^{\langle 2\rangle} = \varepsilon_{xx}^{\langle 1\rangle}\varepsilon_{xx}^{\langle 5\rangle} - \varepsilon_{xx}^{\langle 2\rangle}\varepsilon_{xx}^{\langle 4\rangle} + \int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 3\rangle} d\varepsilon_{xx}^{\langle 3\rangle}\\
&\qquad = \varepsilon_{xx}^{\langle 1\rangle}\varepsilon_{xx}^{\langle 5\rangle} - \varepsilon_{xx}^{\langle 2\rangle}\varepsilon_{xx}^{\langle 4\rangle} + \tfrac{1}{2}(\varepsilon_{xx}^{\langle 3\rangle})^2,
\end{aligned}$$

or, concisely,

$$\begin{aligned}
\int_0^{\varepsilon_{xx}} \varepsilon_{xx}^{\langle 2(n-1)\rangle} d\varepsilon_{xx} &= \varepsilon_{xx}^{\langle 1\rangle}\varepsilon_{xx}^{\langle 2(n-1)-1\rangle} - \varepsilon_{xx}^{\langle 2\rangle}\varepsilon_{xx}^{\langle 2(n-1)-2\rangle} + \cdots + (-1)^{n-1}\varepsilon_{xx}^{\langle n-2\rangle}\varepsilon_{xx}^{\langle n\rangle} + (-1)^n \tfrac{1}{2}(\varepsilon_{xx}^{\langle n-1\rangle})^2\\
&= \sum_{m=1}^{n-2}\big((-1)^{m+1}\varepsilon_{xx}^{\langle m\rangle}\varepsilon_{xx}^{\langle 2(n-1)-m\rangle}\big) + (-1)^n \tfrac{1}{2}(\varepsilon_{xx}^{\langle n-1\rangle})^2,
\end{aligned}$$

which is valid for $n \geq 3$, we conclude that the strain energy $u_n$ at a point is $u_n = u_1 + u_2 + u_3$, where the $u_i$ are given by (13).

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C. W. LIM: bccwlim@cityu.edu.hk
*Department of Building and Construction, City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong*

Y. YANG: yanyang6@student.cityu.edu.hk
*Department of Building and Construction, City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong*

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