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Mathematical Modelling of Rotating Single-walled Carbon Nanotubes used in Nanoscale Rotational Actuators

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ABSTRACT

A rotating single-walled carbon nanotube (SWCNT) is modelled as an Euler-Bernoulli beam using the non-local/non-classical continuum mechanics. These rotating SWCNTs are used in nanoscale rotational actuators. The mathematical model has been used to study the wave behaviour in rotating SWCNTs. The governing partial differential equation for a uniform rotating beam is derived incorporating the non-local scale effects. The spatial variation in centrifugal force has been modelled in an average sense. Even though this averaging seems to be a crude approximation, one can use this as a powerful model in analysing the wave dispersion characteristics of the rotating CNTs. Spectrum and dispersion curves as a function of rotating speed and non-local scaling parameter were obtained. It has been shown that the dispersive flexural wave tends to behave non-dispersively at very high rotation speeds. The numerical results have been simulated for a rotating SWCNT as a waveguide.

Keywords: Carbon nanotubes, wave number, rotational speeds, wave frequency, centrifugal force, dispersion, non-local elasticity, group speed, phase speed

1. INTRODUCTION

Carbon nanotubes were first observed and identified as such by Iijima using transmission electron microscopy in 1991[1]. Nanotubes are cylindrical molecules which consist several concentric sheets of graphene (multi-walled carbon nanotubes - MWCNT). Since the discovery by Iijima, research on carbon nanotubes has become a paramount activity. First their geometry was studied and it was observed that their diameters can range from a few to hundreds of nanometers, and their length, from a few to tens of micrometers[2]. The nanotubes are promising materials in a number of new areas. These include molecular electronics where the nanotubes can be used both for wiring and as electronic devices after modification of the nanotube itself. These can also be used as parts of mechanical devices at the nanoscale such as the shaft of nanomotors[3]. Moreover, their high strength and flexibility are exploited to reinforce materials such as cement. Many production methods have been developed such as the laser vapourisation method combined with transition metal catalyst[4] or the carbon arc method[5]. Nowadays, dozens of companies have become specialised in the production of single- and multi-walled carbon nanotubes. They can produce up to hundreds of grams of SWNTs per day and hundreds of kilograms of MWNTs. Forecasts predict that global demand for nanotubes will expand rapidly[6]. Flat-panel displays for both computers and televisions, will be the first widely commercialised application of these carbon nanotubes.

It was observed that there is a wide variety of carbon nanotubes[2]. Their diameters vary between 0.7 nm and 10 nm, though most of the observed tubes have diameters < 2 nm. The length of single-walled nanotubes goes[7] from a few nm up to 20 cm. Moreover nanotubes can be chiral or achiral. These varieties of SWNTs come from the fact that the nanotubes are constructed by the folding of a graphite plane on itself, and have many ways of folding.

Experiments were conducted to study the rotational motion of concentric nanotubes. In particular, Fennimore[3], *et al.* (Fig. 1(a)) and Bourlon[8], *et al.* (Figs 1(b) & 1(c)) built the

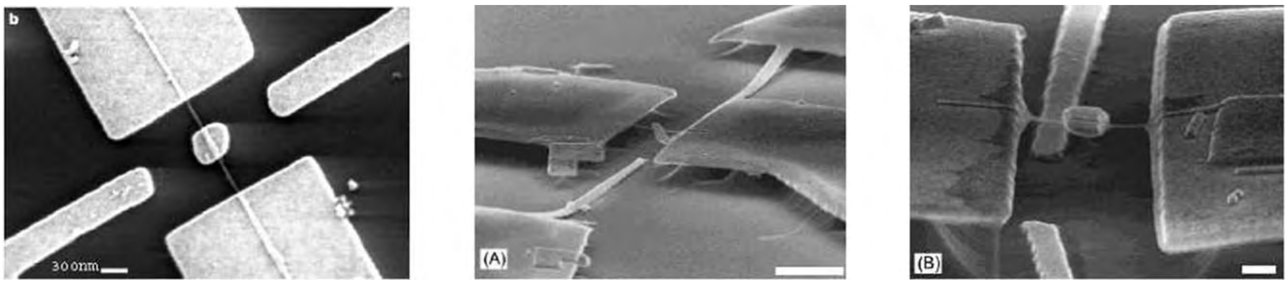

Figure 1. Nanoscale rotational actuators based on nanotubes built by: (a) Fennimore[3], *et al.* (b) & (c) Bourlon[8], *et al.*

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first actuators based on multi-walled nanotubes. Both systems were based on a multi-walled nanotube with edges fixed on two anchor pads. A plate was fixed on the outer shell and which could be rotated with electric fields. The multi-walled nanotube serves as the shaft for this rotary motion. As for the translational oscillatory motion, no wear or fatigue was observed during the rotation. Unfortunately the rotational frequency and dissipation rates could not be measured in these experiments. Recently, Kral and Sadeghpour[9] showed the possibility to spin nanotubes with circularly polarised light, further motivating the usage of nanotubes as possible axis of rotation at the nanoscale. However, no systematic analytical and numerical studies of rotation have yet been carried out, except the work of Zhang[11], *et al.* where non-equilibrium molecular dynamics simulations were carried out to calculate the energy dissipation rate during the rotational motion. In their work, the usage of the thermostat would however add dissipation which is not intrinsic to the system. In the present work, CNT rotating about an axis perpendicular to its longitudinal axis has been considered for the analysis. These types of nanosystems have many applications in the field of nano instrumentation.

The length scales associated with nanostructures like CNTs are such that to apply any classical continuum techniques, the author needs to consider the small length scales such as lattice spacing between individual atoms, surface properties, grain size etc. This makes a physically consistent classical continuum model formulation very challenging. The Eringen's non-local elasticity theory[12-14] is a useful tool in treating phenomena whose origins lie in the regimes smaller than the classical continuum models. In this theory, the internal size or scale could be represented in the constitutive equations simply as material parameters. Such a non-local continuum mechanics has been widely accepted and has been applied to many problems including wave propagation, dislocation, crack problems, etc[17]. Recently, there has been great interest in the application of non-local continuum mechanics for modelling and analysis of CNTs.

Ultrasonic wave propagation analyses of CNTs are relevant due to their various applications[18] which include sensing superconductivity, transport and optical phenomena. CNTs can have interesting waveguide properties at very high frequencies in the order of up to Tera-Hertz (THz). At such high frequencies, continuum model-based finite element type methods cannot be adopted due to their limitation of the element size wrt the wavelength, which is very small at such frequencies. Lattice dynamics for direct observation of phonons[19,20] and spectral finite element type method are more efficient and consistent to analyse such situation[16]. With these theories and methods of analyses, brings out several interesting features of high frequency ultrasonic wave propagation in rotating CNTs, which are not observed in macro-scale structures. In the author's previous works[22-29], only non-rotating CNTs and graphene sheets were considered for the analysis of wave dispersion.

In the present study the wave dispersion characteristics of a rotating SWCNT have been studied using the spectral analysis. The rotating SWCNT is modelled as a Euler-Bernoulli beam. The governing partial differential equation for a uniform rotating beam has been derived incorporating the non-local scale effects and the variable coefficient for the centrifugal term is replaced by the maximum centrifugal force. The rotating beam problem is now transformed to a case of beam subjected to an axial force. Even though this averaging seems to be a crude approximation, one can use this as a powerful model in analysing the wave dispersion characteristics of the rotating CNTs.

2. MATHEMATICAL FORMULATION

2.1 Theory of Non-local Elasticity

This theory assumes that the stress state at a reference point x in the body is regarded to be dependent not only on the strain state at x but also on the strain states at all other points x' of the body. The most general form of the constitutive relation in the non-local elasticity type representation involves an integral over the entire region of interest. The integral contains a non-local kernel function, which describes the relative influences of the strains at various locations on the stress at a given location. The constitutive equations of linear, homogeneous, isotropic, non-local elastic solid with zero body forces are given by[12,13]

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

$$\sigma_{ij}(x) = \int_V \alpha(|x - x'|, \xi)\sigma^c_{ij}(x')dV(x') \tag{2}$$

$$\sigma^c{}_{ij} = C_{ijkl}\varepsilon_{kl} \tag{3}$$

$$\varepsilon_{ij}(x') = \frac{1}{2}\left(\frac{\partial u_i(x')}{\partial x_{j'}} + \frac{\partial u_j(x')}{\partial x_{i'}}\right) \tag{4}$$

Equation (1) is the equilibrium equation, where $\sigma_{ij,i}$, ρ, f_j, u_j are the stress tensor, mass density, body force density and displacement vector at a reference point x in the body, respectively, at time t. Equation (3) is the classical constitutive relation where $\sigma^c{}_{ij}(x')$ is the classical stress tensor at any point x' in the body, which is related to the linear strain tensor $\varepsilon_{ij}(x')$ at the same point. Equation (4) is the classical strain-displacement relationship. The only difference between Eqns. (1)-(4) and the corresponding equations of classical elasticity is the introduction of Eqn. (2), which relates the global (or non-local) stress tensor $\sigma_{ij,i}$ to the classical stress tensor $\sigma^c{}_{ij}(x')$ using the modulus of non-localness. The modulus of non-localness or the non-local modulus $\alpha(|x - x'|, \xi)$ is the kernel of the integral Eqn. (2) and contains parameters which correspond to the non-localness[13]. A dimensional analysis of Eqn. (2) clearly shows that the non-local modulus has dimensions of $(length)^{-3}$ and so it depends on a characteristic length ratio a/ℓ where a is an internal characteristic length (lattice parameter, size of grain, granular distance, etc.) and ℓ is an external characteristic length of the system (wavelength, crack length, size or dimensions of sample, etc.). Therefore the non-local modulus can be written in the following form:

$$\alpha = \alpha(|x - x'|, \xi), \xi = \frac{e_0 a}{\ell} \tag{5}$$

where e_0 is a constant appropriate to the material and has to be determined for each material independently[13].

Making certain assumptions[13], the integro-partial differential equations of non-local elasticity can be simplified to partial differential equations. For example, Eqn. (2) takes the following simple form:

$$\left(1 - \xi^2 \ell^2 \nabla^2\right)\sigma_{ij}(x) = \sigma^c{}_{ij}(x) = C_{ijkl}\varepsilon_{kl}(x) \tag{6}$$

where C_{ijkl} is the elastic modulus tensor of classical isotropic elasticity and ε_{ij} is the strain tensor. where ∇^2 denotes the second-order spatial gradient applied on the stress tensor σ_{ij} and $\xi = e_0 a / \ell$.

A method of identifying the small scaling parameter e_0 in the non-local theory is not known yet. As defined by Eringen[13], e_0 is a constant appropriate to each material. Eringen proposed e_0=0.39 by the matching of the dispersion curves via non-local theory for plane wave and Born-Karman model of lattice dynamics at the end of the Brillouin zone (ka=π), where a is the distance between atoms and k is the wavenumber in the phonon analysis[13]. On the other hand, Eringen proposed e_0=0.31 in his study[14] for Rayleigh surface wave via non-local continuum mechanics and lattice dynamics.

2.2 Governing Differential Equations of Rotating SWCNTs

Nanotubes are central to new rotating devices such as miniature motor. A rotating CNT can be represented as a cantilever beam having displacements perpendicular to the plane of rotation. Considering the elementary Euler-Bernoulli theory of beams, the axial and transverse displacement fields of a rotating beam can be represented

$$u(x, y, z, t) = u^0 - z w_{,x} \tag{7}$$

$$w(x, y, z, t) = w(x, t) \tag{8}$$

where w is transverse displacements of the point (x, 0) on the middle plane (i.e., z = 0) of the beam. The only non-zero strain of the Euler–Bernoulli beam theory, accounting for the von Kármán nonlinear strain is

$$\varepsilon^{(xx)} = u_{,x} = u^0_{,x} - z w_{,xx} \tag{9}$$

This is also called as bending strain. The equations of motion of the Euler-Bernoulli beam theory are given by

$$Q_{,x} = \rho A \ddot{u}^0 \tag{10}$$

$$M_{,xx} + \left(T(x) w_{,x}\right)_{,x} = \rho A \ddot{w} \tag{11}$$

where

$$Q = \int_A \sigma^{(xx)} dA, M = \int_A z\sigma^{(xx)} dA \tag{12}$$

and $\sigma^{(xx)}$ is the axial stress on the $yz-$ section in the direction of x, Q is the axial force, M is the bending moment and $T(x)$ is the axial force due to centrifugal stiffening and is given as

$$T(x) = \int_x^L \rho A \Omega^2 x dx \tag{13}$$

where ρ is the mass density, A is the beam cross section area and Ω is the rotation speed.

Using Eqn. (6), stress resultants of Euler Bernoulli beam theory have been expressed in terms of the strains in that theory. As opposed to the linear algebraic equations between the stress resultants and strains in a local theory, the non-local constitutive relations lead to differential relations involving the stress resultants and the strains. In the following, these relations for homogeneous isotropic beams are presented. The non-local constitutive relations in Eqn. (6) take the following special form for beams:

$$\sigma^{(xx)} - (e_0 a)^2 \sigma^{(xx)}_{,xx} = E\varepsilon^{(xx)} \tag{14}$$

where E is the Young's modulus of the beam. Using Eqns (12) and (14), one has

$$Q - (e_0 a)^2 Q_{,xx} = EA u_{,x} \tag{15}$$

$$M - (e_0 a)^2 M_{,xx} = EI\kappa_e \tag{16}$$

where $I = \int_A z^2 dA$ is the moment of inertia of the beam cross section and $k_e = -w_{xx}$ is the bending strain of the beam.

Using non-local constitutive relations and the equations of motion presented, the moment can be expressed in terms of the generalised displacements, by substituting Eqn. (16) into Eqn. (11), as

$$M = -Elw_{,xx} + (e_0 a)^2 \left\lfloor \rho A \ddot{w} - (T((x) w_{,x})_{,x} \right\rfloor \tag{17}$$

Substituting M from Eqn. (17) into Eqn. (11), the equation of motion of rotating non-local Euler beams is obtained as

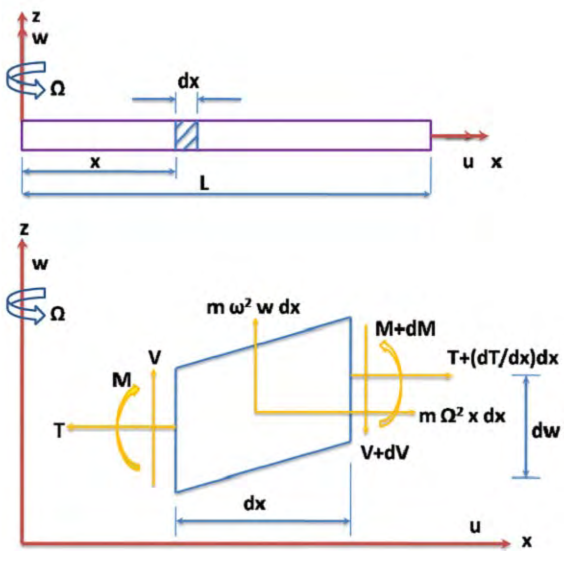

Figure 2. Forces acting on an incremental length *dx* of the rotating beam.

$$-EIw_{,xxxx} + (e_0 a)^2 \left\lfloor \rho A\ddot{w} - (T((x)w_{,x})_{,x} \right\rfloor_{,xx} + (T((x)w_{,x}) = \rho A\ddot{w} \tag{18}$$

A uniform rotating beam is assumed and $T(x)$ is replaced by the maximum force at the root, i.e., at $x = 0$

$$T_{\max} = \int_0^L \rho A\Omega^2 x dx = \frac{\rho A\Omega^2 L^2}{2} \tag{19}$$

This allows to represent governing equation as a constant coefficient non-local partial differential equation. Finally, the non-local governing differential equation for transverse displacement ($w(x,t)$) of a rotating cantilever beam is derived as

$$-EIw_{,xxxx} - T_{\max} w_{,xx} + T_{\max} (e_0 a)^2 w_{,xxxx} + \rho A\ddot{w} - \rho A(e_0 a)^2 \ddot{w}_{,xx} = 0 \tag{20}$$

This equation reduces to classical one, once the non-local scale parameter is neglected.

3. ULTRASONIC WAVE DISPERSION ANALYSIS IN ROTATING SWCNTS

For analysing the dispersion characteristics of waves in SWCNTs, a harmonic type of wave solution for the displacement field $w(x,t)$ is assumed and it can be expressed in complex form[12,13] as

$$w(x,t) = \sum_{n=1}^{N} \hat{w}(x,\omega_n) e^{-j(kx-\omega_n t)} \tag{21}$$

where $\hat{w}(x,\omega_n)$ is the frequency domain amplitude of the flexural deformation of CNTs, k is the wavenumber and ω_n is the angular frequency of the wave motion at n^{th} sampling point, N is the Nyquist frequency and $j = \sqrt{-1}$. Eliminating the time variable from Eqn. (20) using the above spectral approximation of the displacement gives,

$$EI\hat{w}^{iv} - T_{\max} \hat{w}^{ii} + T_{\max} (e_0 a)^2 C^{iv} - \rho A\omega^2 \hat{w} + \rho A(e_0 a)^2 \omega^2 \hat{w}^{ii} = 0 \tag{22}$$

For the sake of simplicity in the analysis, this equation is expressed in a non-dimensional form. New variables are defined as

$$\tilde{x} = \frac{x}{L};\ \hat{w} = \frac{\tilde{w}}{L};\ \frac{d\hat{w}}{dx} = \frac{d\tilde{w}}{d\tilde{x}};\ L\frac{d^2\hat{w}}{dx^2} = \frac{d^2\tilde{w}}{d\tilde{x}^2};$$
$$L^2\frac{d^3\hat{w}}{dx^3} = \frac{d^3\tilde{w}}{d\tilde{x}^3}; L^3\frac{d^4\hat{w}}{dx^4} = \frac{d^4\tilde{w}}{d\tilde{x}^4};\ \tau = \frac{e_0 a}{L} \tag{23}$$

The non-dimensional form of the Eqn.(22) is

$$EI\frac{1}{L^3}\frac{d^4\tilde{w}}{d\tilde{x}^4} - T_{\max}\frac{1}{L}\frac{d^2\tilde{w}}{d\tilde{x}^2} + T_{\max}(e_0 a)^2 \frac{1}{L^3}\frac{d^4\tilde{w}}{d\tilde{x}^4}$$
$$-\rho A\omega^2 L\tilde{w} + \rho A(e_0 a)^2 \omega^2 \frac{1}{L}\frac{d^2\tilde{w}}{d\tilde{x}^2} = 0 \tag{24}$$

Rearranging and defining a new variable

$$\omega_{str} = \frac{1}{L^2}\sqrt{\frac{EI}{\rho A}} \tag{25}$$

Equation (24) changes to the differential equation of constant coefficients type, it has the solution of the form $\tilde{w} = \tilde{W}e^{-jkx}$, on substituting, this solution (since, for nontrivial solution $\tilde{W} \neq 0$) is obtained as follows:

$$\left[1 + \tau^2 \frac{1}{2}\left(\frac{\Omega}{\omega_{str}}\right)^2\right]k^4 + \left[\frac{1}{2}\left(\frac{\Omega}{\omega_{str}}\right)^2 - \tau^2\left(\frac{\omega}{\omega_{str}}\right)^2\right]k^2 - \left(\frac{\omega}{\omega_{str}}\right)^2 = 0 \tag{26}$$

where k is the wavenumber. This is the dispersion/characteristic equation of the rotating uniform beams. One can solve for the wavenumbers. The wavenumbers are mainly a function of the non-local scaling parameter ($e_0 a$), rotational speed of the beam (Ω), and the wave circular frequency. The corresponding wave speeds, namely, phase-speed $C_p = \mathrm{Re}\left(\frac{\omega}{k}\right)$ and group-speed $C_g = \mathrm{Re}\left(\frac{\partial\omega}{\partial k}\right)$, are obtained from Eqn. (26).

4. NUMERICAL RESULTS AND DISCUSSION

For numerical experiments, a (5,5) SWCNT is considered and the diameter of the SWCNT is d = 0.675 nm, length L = 10 d, Young's modulus E = 5.5 TPa and the density ρ = 2300 kg/m^3.

The spectrum curves (i.e., wavenumber *vs* wave frequency) for the rotating SWCNT are shown in Fig. 3 for different values of the rotational speed Ω for $\tau = e_0 a / L = 0$ (i.e., local elasticity calculation). It can be seen that for non-rotating CNT (i.e., $\Omega/\omega_{str} = 0$), the flexural wavenumber shows a nonlinear variation with wave frequency, i.e., the waves will change their shape as these propagate. As the rotational speed of the CNT increases, the wavenumbers are non-dispersive in nature as shown in Fig. 3. It means that the waves will not change their shapes as these propagate in the medium. Also, the wavenumber shows an inverse dependence on rotation speed. For a non-rotating CNT, the spectrum relation is dispersive in nature. But for a rotating beam, at higher speeds, the above nonlinear relation shifts to a linear nature due to the relatively

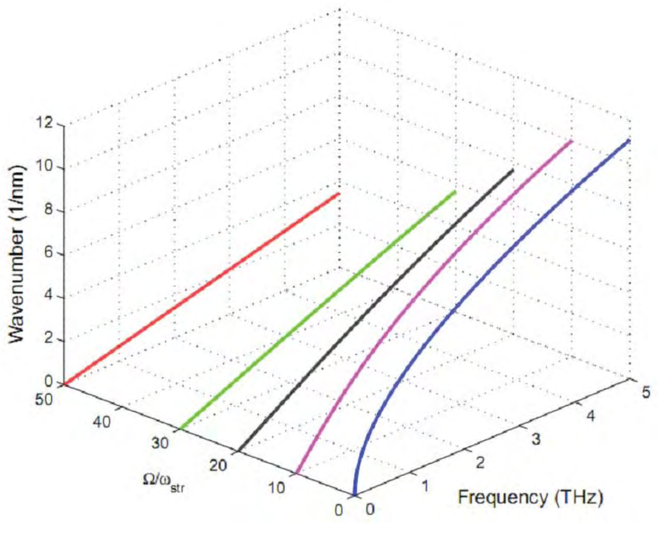

Figure 3. Wavenumber dispersion in a rotating CNT for $\tau = e_0 a / L = 0$ for different values of Ω/ω_{str} .

negligible contribution from the ω term, especially for lower values of ω. That is, the variation of k is dominated by the centrifugal force term at high Ω/ω_{str} .

Figures 4(a) to 4(b), show the spectrum curves for rotating and non-rotating CNTs for various values of the non-local scaling parameter. Figure 4(a) shows that as one moves from local elasticity to non-local elasticity solution, the spectrum curve becomes linear at higher values of the wave frequency. The wavenumbers also increases as the non-local scaling parameter increases. The matching of local and non-local solutions is limited only up to < 0.2 THz frequency. After this frequency, the difference between the wavenumbers predicted is very large. If the rotational speed of the CNT increases from $\Omega/\omega_{str} = 0$ to $\Omega/\omega_{str} = 10$ (Fig. 4(b)), the spectrum curve is slightly nonlinear as compared to nonrotating case. The wavenumbers obtained from local and non-local cases is same upto 0.45 THz frequency. The wavenumbers are showing an increase in tendency as the non-local parameter increases. If the rotational speed of the CNT increases to very high values like $\Omega/\omega_{str} = 50$ and 100, the local and non-local calculations are almost similar upto 1.6 THz and 2.5 THz frequencies, respectively (see Figs 4(c) & 4(d)). As the rotational speed of the CNT increases to very high values, the non-local scaling parameter effect on the spectrum curves is negligible. It means that if the CNT rotates at very high speeds, the local elasticity and non-local elasticity calculations give almost similar spectrum relations. It can also be observed that as the rotational speed of the CNT increases, the wavenumbers become very small and the dispersive nature changes to non-dispersive nature (Fig. 4).

The phase-speed and group-speed dispersions of the rotating CNT are shown in Fig. 5, obtained from the local elasticity calculations (i.e., $\tau = 0$). Thick lines represent the phase-speed variations and the thin lines show the group-speed variations. It can be seen that the phase-speed of the

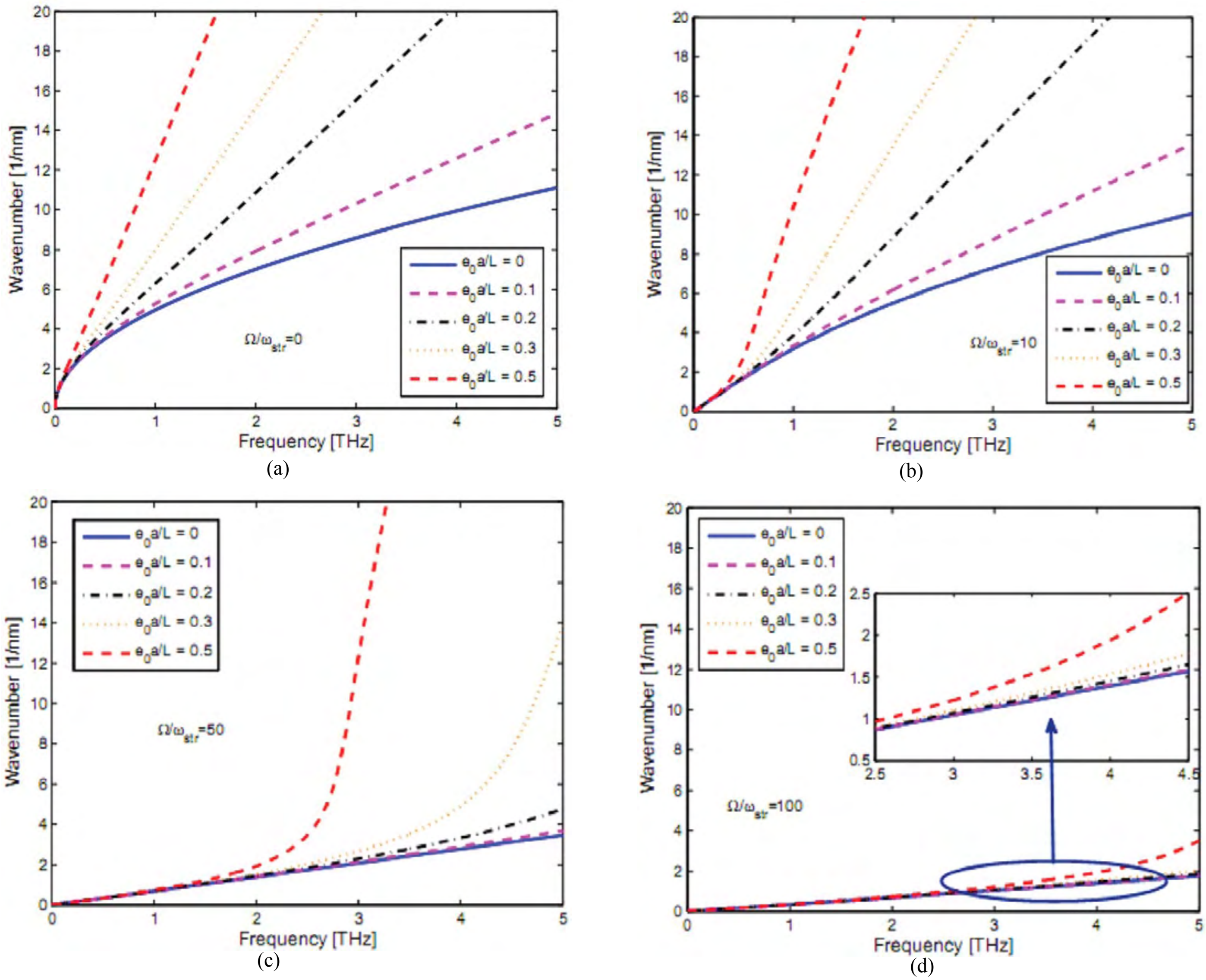

Figure 4. Wave dispersion for various values of τ = 0, 0.1, 0.2, 0.3, 0.5. For (a) $\Omega/\omega_{str} = 0$; (b) $\Omega/\omega_{str} = 10$; (c) $\Omega/\omega_{str} = 50$, and (d) $\Omega/\omega_{str} = 100$.

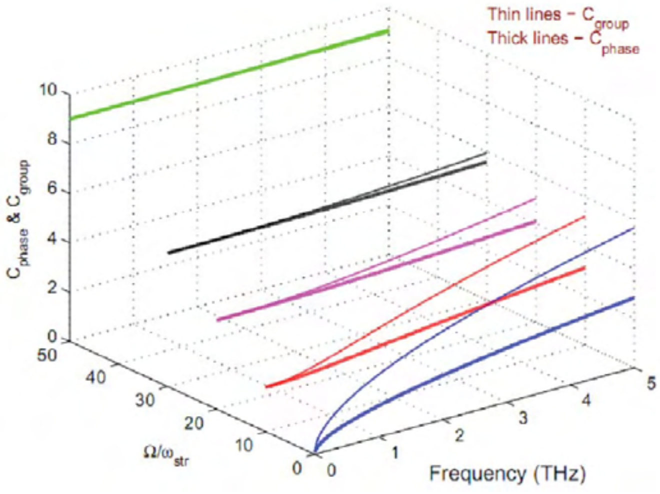

Figure 5. Phase-speed (thick lines) and group-speed (thin lines) dispersions in rotating nanobeam for $\tau = 0$ for different values of $\Omega/\omega_{str} = 0$.

rotating CNTs is higher than the group speed. Because of the nonlinear relation of the wavenumber with wave frequency, for non-rotating CNTs, the phase and group speeds also show a nonlinear variation with frequency. As the rotational speeds of the CNT increase to higher values, both the phase-speed and group-speed will saturate to a constant velocity, because of the linear variation of the wavenumber with wave frequency. The difference between the phase and group speeds of the rotating CNTs is negligible at higher rotational speeds, as shown in Fig. 5, which is a characteristic of any non-dispersive system. As the limiting case, these become equal and become constant for all wave frequencies. For a non-rotating beam, both phase-speed and group-speeds are dispersive and show that the speeds approach infinity for very high frequencies. This unreasonable limit is due to the limitation of Euler-Bernoulli beam theory.

Figure 6 shows the phase-speed and group-speed variations with both the wave frequency and the non-local scaling parameter for rotating and non-rotating CNTs. Figure 6(a) shows that for a non-rotating CNT, the phase and group speeds will decrease as the non-local scaling parameter

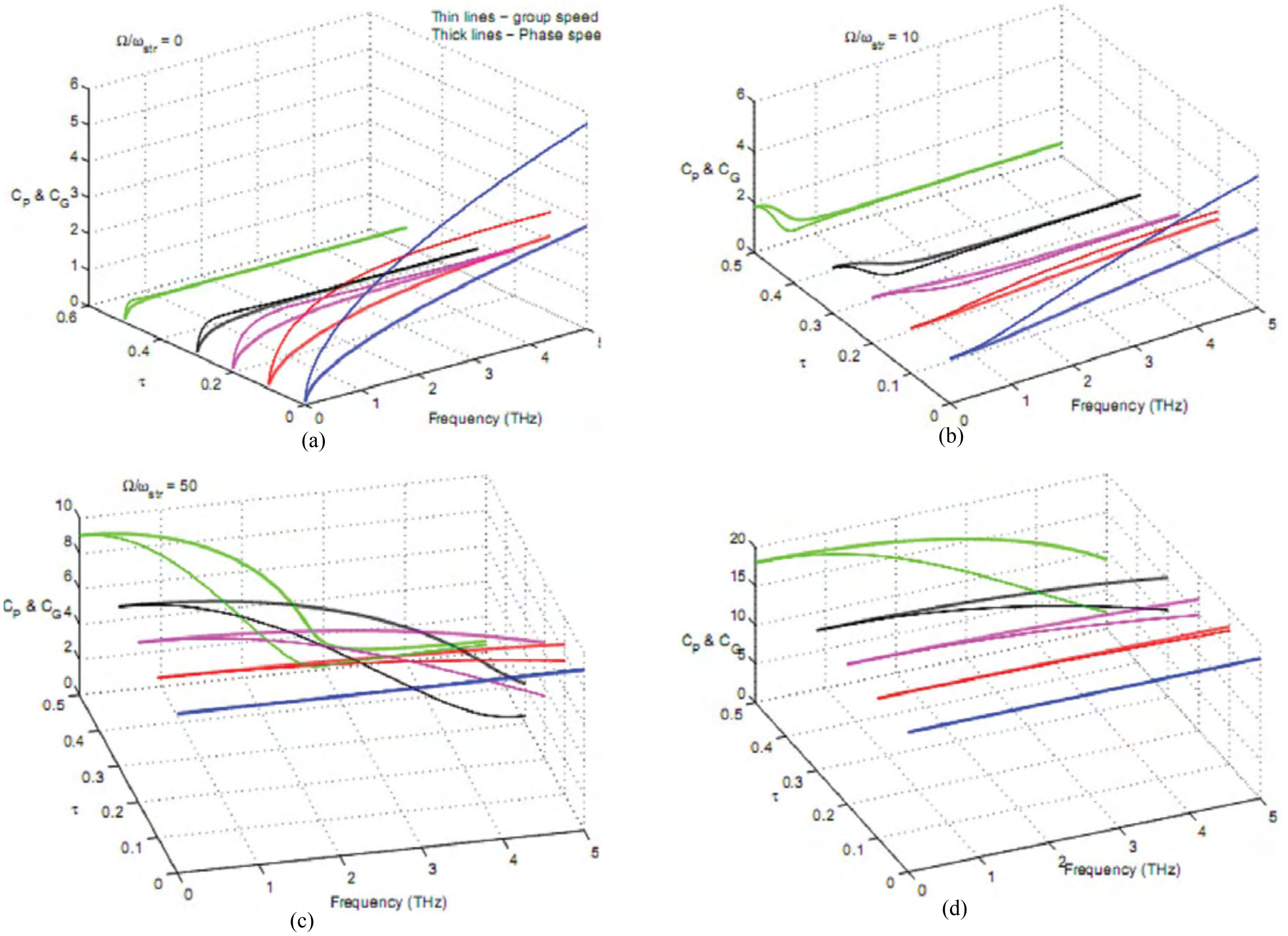

Figure 6. Phase-speed (thick lines) and group-speed (thin lines) dispersions in rotating nanobeam for different values of Ω/ω_{str}. Here (a) $\Omega/\omega_{str} = 0$, (b) $\Omega/\omega_{str} = 10$, (c) $\Omega/\omega_{str} = 50$, and (d) $\Omega/\omega_{str} = 100$.

increases, because the wavenumbers are increasing with increase in τ (Fig. 4). Also, the difference between the phase-speed and group-speeds dips at higher values of τ. As the rotational speed of the CNT increases, both phase and group speeds will also increase, as shown in Figs 6(b)-6(d). For small rotational speeds and large values of τ, both group speeds show a decrease in nature at smaller frequencies and these become constant at higher wave frequencies. Such a difference will also vanish at higher rotational speeds, as shown in Fig. 6(d). On the other hand, one more interesting feature of the non-locality is that, the difference between both the wave speeds is considerable at smaller rotational speeds and τ and also at the higher rotational speeds and τ and it can be clearly seen from Fig. 6.

5. CONCLUSIONS

The wave dispersion characteristics of a rotating SWCNT have been studied using the spectral analysis. The rotating SWCNT is modelled as a Euler-Bernoulli beam. The governing partial differential equation for a uniform rotating beam is derived incorporating the non-local scale effects and a powerful model has been derived in analysing the wave dispersion characteristics of the rotating CNT. Some of the features of the wave behaviour in rotating CNTs are observed. Such observations are helpful in designing the nanomotors, actuator, and the other CNT-based rotational nanodevices.

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