Nonlocal Flexural Wave Propagation in an Embedded Graphene

S. Narendar and S. Gopalakrishnan

Abstract—This paper presents the strong nonlocal scale effect on the terahertz flexural wave dispersion characteristics of a monolayer graphene sheet, which is embedded in elastic medium. The graphene is modeled as an isotropic plate of one atom thick. The chemical bonds are assumed to be formed between the GSs and the elastic medium. The polymer matrix is described by a Pasternak foundation model. The elastic foundation is approximated as a series of closely spaced, mutually independent, vertical linear elastic springs where the foundation modulus is assumed equivalent to stiffness of the springs. Nonlocal governing equation of motion is derived and wave propagation analysis is performed using spectral analysis. The present analysis shows that the flexural wave dispersion in graphene obtained by local and nonlocal elasticity theories is quite different. From this analysis we show that the elastic matrix highly affects the flexural wave mode and it rapidly increases the frequency band gap of flexural wave. The nonlocal elasticity calculation shows that the wavenumber escapes to infinite at certain frequency and the corresponding wave velocity tends to zero at that frequency indicating localization and stationary behavior. This behavior is captured in the spectrum and dispersion curves. It has been shown that the cut-off frequency of flexural wave not only depends on the axial wavenumber but also on the nonlocal scaling parameter. The effect of y-directional wavenumber and nonlocal scaling parameter on the cut-off frequency is also captured in the present work.

Keywords-Graphene, Wavenumber, Nonlocal Elasticity, Pasternak Foundation, Phase Speed, Cut-off Frequency, Escape Frequency.

I. INTRODUCTION

N recent years, nanostructured materials have spurred considerable interest in the materials community because of their potential for large gains in mechanical and physical properties as compared to standard structural materials. Since controlled experiments in nanoscale are difficult and molecular dynamics simulation are expensive and formidable especially for large scale systems. Thus, modified continuum models have been widely and successfully used to study mechanical behavior of nanostructures like carbon nanotubes (CNTs), graphene sheets (GSs), nanofibres/wires, etc [1].Since the focus of this work is on two-dimensional nanostructures. 2D-

S. Gopalakrishnan is with Department of Aerospace Engineering, Indian Institute of Science, Bangalore 560 012 INDIA.

E-mail: krishnan@aero.iisc.ernet.in.

nanostructures (here GSs) have stimulated a great deal of interest due to their importance in fundamental scientific research and potential technological applications in nanoelectronic, nano-optoelectronic and nano-electro-mechanical systems..

Single-layered graphene sheets (SLGSs) are consisting of a number of carbon atoms which are interconnected via covalent bonds in the honeycomb lattice. The graphene is of single atom thick in size and is the basic structural element of all other graphitic materials including graphite, carbon nanotubes (CNTs), and fullerenes. After GSs are reported to be effectively extracted from graphite [2] its potential applications as an industrial material is expected. A SLGS or a multilayered graphene sheets (MLGSs) are found as embedded in elastic medium, such as in polymer composites. This is done for enhancement of strength of the parent material.

Nanotechnology's small scale makes the applicability of classical or local continuum models, such as beam, shell and plate models, questionable. Classical continuum models do not admit intrinsic size dependence in the elastic solutions of inclusions and in homogeneities. At nanometer scales, however, size effects often become prominent, the cause of which needs to be explicitly addressed due to an increasing interest in the general area of nanotechnology [3]. Sun et al. [4] indicated the importance of a semi-continuum model in analyzing nanomaterials after pointing out the limitations of the applicability of classical continuum models to nanotechnology. In their semi-continuum model for nanostructured materials with plate like geometry, material properties were found completely dependent on the thickness of the plate structure contrary to classical continuum models. The modeling of such a size-dependent phenomenon has become an interesting research subject in this field [5]. It is thus concluded that the applicability of classical continuum models at very small scales is questionable, since the material microstructure, such as lattice spacing between individual atoms, becomes increasingly important at small size and the discrete structure of the material can no longer be homogeneities into a continuum. Therefore, continuum models need to be extended to consider the scale effect in nanomaterial studies. This can be accomplished through proposing nonlocal continuum mechanics models.

Nonlocal elasticity theory [6, 7] was proposed to account for the scale effect in elasticity by assuming the stress at a reference point to be a function of strain field at every point in the body. This way, the internalize scale could be

Manuscript received October 17, 2011: Revised version received xx xx XXXX.

S. Narendar is with the Defence Research and Development Laboratory, Kanchanbagh, Hyderabad 500 058 INDIA. Phone: +91-88-9762 5977; fax: +91-40-2434 2309; e-mail: nanduslns07@gmail.com or snarendar@aero.iisc.ernet.in.

simply considered in constitutive equations as a material parameter only recently has the nonlocal elasticity theory been introduced to nanomaterial applications. Peddiesonet al. [8] applied nonlocal elasticity to formulate a nonlocal version of the Euler-Bernoulli beam model and concluded that nonlocal continuum mechanics could potentially play a useful role in nanotechnology applications. Inspired by the above conclusion on the applicability of nonlocal elasticity to nanotechnology, nonlocal Euler-Bernoulli beam and shell models have been employed to study CNTs and GSs mechanical behaviors by other researchers [9-13].

Ultrasonic wave propagation analysis of graphene sheets is relevant due to their various applications which include sensing superconductivity, transport and optical phenomena. Graphene has 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 with respect to the wavelength, which is very small at such frequencies. Lattice dynamics for direct observation of phonons [14, 15] and spectral finite element type method are more efficient and consistent to analyze such situation [16, 17]. With these theories and method of analysis, the present study brings out several interesting features of high frequency ultrasonic wave propagation in GSs, which are not observed in macro-scale structures.

Most of the studies on vibration and buckling of nanoplates are carried out on single-layered GSs and multilayered graphene sheets. Graphene is a new class of twodimensional carbon nanostructure which holds great promise for the vast applications in many technological fields. It would be one of the prominent new materials for the next generation nano-electronic devices. Reports related to its applications as strain sensor, mass and pressure sensors, atomic dust detectors, enhancer of surface image resolution are observed. After graphene sheets are reported to be successfully extracted from graphite, its potential applications as an industrial material is expected. Consequently interest is drawn towards research of graphene in the field of physics, material science and engineering. Some vibration studies on graphene nanosheets are reported recently. However studies on wave propagation aspect of graphene sheets are minuscule in numbers. GSs can have interesting waveguide properties at very high frequencies in the order of 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 with respect to the wavelength, which is very small at such frequencies. Lattice dynamics for direct observation of phonons and spectral finite element type method are more efficient and consistent to analyze such problem.

In wave mechanics of nanostructures, one important outcome of the nonlocal elasticity is the realistic prediction of the dispersion curve i.e., frequency-wavenumber/wavevector relation. As shown in Eringen [7], the dispersion relation

$$\frac{\omega}{C_1 k} = \left(1 + (e_0 a)^2 k^2\right)^{-1/2}$$

where $e_0 a$ = nonlocality parameter, closely matches with the

Born–Karman model dispersion

$$\frac{\omega a}{C_1} = 2\sin\left(\frac{ka}{2}\right)$$

when $e_0 = 0.39$ is considered. However, among the two natural conditions at the mid-point and end of the first Brillouin zone:

$$\left. \frac{d\omega}{dk} \right|_{k=0} = C_1; \left. \frac{d\omega}{dk} \right|_{k=\frac{\pi}{a}} = 0$$

these relations satisfy only the first one. It was suggested that two-parameter approximation of the kernel function will give better results. So, the one parameter (only e_0a) non-local kernel will never be able to model the lattice dynamics relation and it is necessary to use the bi-Helmholtz type equation with two different coefficients of non-locality to satisfy all the boundary conditions.

It is to be noted that the simple forms of the group and phase velocities that exist for isotropic materials permitted to tune the non-locality parameters so that the lattice dispersion relation is matched. Further, by virtue of the Helmholtz decomposition, only one-dimensional Brillouin zone needs to be handled. Although the general form of the boundary conditions, i.e., group speed is equal to phase speed (at k = 0) or zero (at $k = \pi / a$), is still applicable, the expressions are difficult to handle. This is because, the Brillouin zone is really a two-dimensional region where four boundary conditions are involved.

The main objective of the work reported here was to establish a simple and suitable nonlocal continuum based model to investigate the wave dispersion behavior of a SLGS that is embedded in an elastic polymer matrix at Terahertz frequency level. Both Winkler-type and Pasternak-type models are used to simulate the interaction of the GSs with the surrounding elastic medium. A set of explicit formulas is derived for the wavenumbers and the associated wave speeds of GS embedded in polymer matrix. These formulas clearly indicate the influence of surrounding matrix on the wave dispersion behavior. The effects of the nonlocal scale and of the surrounding matrix on the wavenumbers, the associated wave speeds and cut-off frequencies are examined in graphical form.

II. MATHEMATICAL FORMULATION

A. A Review on Nonlocal Elasticity Theory

Nonlocal elastic 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 nonlocal elasticity type representation involves an integral over the entire region of interest. The integral contains a nonlocal 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 body forces are given by [7] INTERNATIONAL JOURNAL OF COMPUTERS Issue 1, Volume 6, 2012

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

$$\sigma_{ij}(x) = \int_{V} \alpha(|x - x'|, \xi) \sigma_{ij}^{c}(x') dV(x')$$
⁽²⁾

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

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

Equation (1) is the equilibrium equation, where σ_{ij} , ho , f_j and u_i 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 $\sigma_{ii}^{c}(x')$ is the classical stress tensor at any point x' in the body, which is related to the linear strain tensor $\mathcal{E}_{kl}(x')$ at the same point. Equation (4) is the classical strain-displacement relationship. The only difference between equations (1)-(4) and the corresponding equations of classical elasticity is the introduction of equation (2), which relates the global (or nonlocal) stress tensor σ_{ii} to the classical stress tensor $\sigma_{ii}^{c}(x')$ using the modulus of nonlocalness. The modulus of nonlocalness or the nonlocal modulus $\alpha(|x-x'|,\xi)$ is the kernel of the integral equation (2) and contains parameters which correspond to the nonlocalness [7]. A dimensional analysis of equation (2) clearly shows that the nonlocal 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 nonlocal modulus can be written in the following form:

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

where e_0 is a constant appropriate to the material and has to be determined for each material independently [7].

Making certain assumptions [7], the integro-partial differential equations of nonlocal elasticity can be simplified to partial differential equations. For example, equation (2) takes the following simple form:

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

where C_{ijkl} is the elastic modulus tensor of classical isotropic elasticity and ε_{ii} 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 nonlocal theory is not known yet. As defined by Eringen [7], e_0 is a constant appropriate to each material. Eringen proposed $e_0 = 0.39$ by the matching of the dispersion curves via nonlocal theory for plane wave and Born-Karman model of lattice dynamics at the end of the Brillouin zone $(ka = \pi)$, where *a* is the distance between atoms and *k* is the wavenumber in the phonon analysis.

B. Nonlocal governing partial differential equation of motion for graphene embedded in elastic medium

A single-layered rectangular GS embedded in an elastic medium (polymer matrix) is considered (see Fig. 1). The chemical bonds are assumed to be formed between the GSs and the elastic medium. The polymer matrix is described by a Pasternak foundation model, which accounts for both normal pressure and the transverse shear deformation of the surrounding elastic medium. When the shear effects are neglected, the model reduces to Winkler foundation model.

The normal pressure or Winkler elastic foundation parameter is approximated as a series of closely spaced, mutually independent, vertical linear elastic springs where the foundation modulus is assumed equivalent to stiffness of the springs. The normal pressure and the incompressible layer that resists transverse shear deformation by Winkler and Pasternak foundation model are expressed as

$$Q_{Winkler} = K_W \ W \tag{7}$$

$$Q_{Pasternak} = K_G w - K_G (w_{,xx} + w_{,yy})$$
(8)

where K_W and K_G denote the Winkler modulus parameter and the shear modulus of the surrounding medium, respectively. Based on Hamilton's principle the equilibrium equations could be obtained in Cartesian coordinates along the length and breadth of the sheet. The two-dimensional nonlocal constitutive relations are also obtained by expressing the bending moments as a function of stress resultants. Using the nonlocal constitutive relations and the moment-stress resultant expressions, nonlocal constitutive relations in terms of displacements are obtained. The obtained stress-resultant displacement equations can be reduced to that of classical plate model when the scale coefficient e_0a is set to zero. Substituting nonlocal moment-resultant displacement relations in to the equilibrium equation we get the final governing equation as INTERNATIONAL JOURNAL OF COMPUTERS Issue 1, Volume 6, 2012

$$C_{11}I_{2}w_{,xxxx} + 2(C_{12} + 2C_{66})I_{2}w_{,xx,yy} + C_{22}I_{2}w_{,yyyy} -J_{0}\mu^{2}(\ddot{w}_{,xx} + \ddot{w}_{,yy}) + J_{2}\mu^{2}(\ddot{w}_{,xxxx} + 2\ddot{w}_{,xx,yy} + \ddot{w}_{,yyyy}) +J_{0}\ddot{w} - J_{2}(\ddot{w}_{,xx} + \ddot{w}_{,yy}) + K_{W}w - K_{W}\mu^{2}(w_{,xx} + w_{,yy}) -K_{G}(w_{,xx} + w_{,yy}) + K_{G}\mu^{2}(w_{,xxxx} + 2w_{,xx,yy} + w_{,yyyy}) = 0 (9)$$

where

 $C_{11} = C_{22} = E / (1 - v^2); C_{12} = C_{21} = vE / (1 - v^2);$

 $C_{66} = 0.5E/(1+\nu)$ and $\mu = e_0 a$. The governing equation (9) reduces to that of the classical plate model when the scale coefficients set to zero. Here $I_2 = \int_{-h/2}^{+h/2} z^2 dz$ and $J_2 = \int_{-h/2}^{+h/2} \rho z^2 dz$.



Fig. 1 Continuum equivalent model of monolayer graphene embedded in elastic medium, here K_W and K_G denote the Winkler modulus parameter and the shear modulus of the surrounding medium, respectively.

C. Ultrasonic flexural wave characteristics of a monolayer graphene sheet embedded in elastic matrix

The wave dispersion formulation begins by assuming a solution of the displacement field. In particular, time harmonic waves are sought and it is assumed that the model is Y-direction (although bounded unbounded in X – direction). Thus the assumed form is a combination of Fourier transform in Y – direction and Fourier transform in time [16, 17]

$$w(x, y, t) = \sum_{n=1}^{N} \sum_{m=1}^{M} \hat{w}(x) e^{-j\eta_m y} e^{j\omega_n t}$$
(10)

where ω_n and the η_m are the circular frequency at *n* th sampling point and the wavenumber in y-direction at the m th sampling point, respectively. The N is the index corresponding to the Nyquist frequency in fast Fourier transform (FFT), which is used for computer implementation of the Fourier transform.

Substituting Eq. (10) in Eq. (9), an ordinary differential equation (ODE) is obtained for the unknown $\hat{w}(x)$

as

$$H_4 \frac{d^4 \hat{w}}{dx^4} + H_2 \frac{d^2 \hat{w}}{dx^2} + H_0 \hat{w} = 0$$
(11)

where

$$H_{4} = C_{11}I_{2} - J_{2}\mu^{2}\omega_{n}^{2} + K_{G}\mu^{2}$$

$$H_{2} = -2(C_{12} + 2C_{66})I_{2}\eta_{m}^{2} + J_{0}\mu^{2}\omega_{n}^{2} - 2J_{2}\mu^{2}\eta_{m}^{2}\omega_{n}^{2}$$

$$+J_{2}\omega_{n}^{2} - K_{W}\mu^{2} - K_{G} - 2K_{G}\mu^{2}\eta_{m}^{2}$$

$$H_{0} = C_{22}I_{2}\eta_{m}^{4} - J_{0}\mu^{2}\omega_{n}^{2}\eta_{m}^{2} - J_{2}\mu^{2}\omega_{n}^{2}\eta_{m}^{4} - J_{0}\omega_{n}^{2}$$

$$-J_{2}\omega_{n}^{2}\eta_{m}^{2} + K_{W} + K_{W}\mu^{2}\eta_{m}^{2} + K_{G}\eta_{m}^{2} + K_{G}\mu^{2}\eta_{m}^{4}$$

Since this ODE is having constant coefficients, its solution can be written as $\hat{w}(x) = \tilde{w}e^{jkx}$, where k is the wavenumber in x – direction, yet to be determined and \tilde{W} is an unknown constant. Substituting this assumed form of \hat{w} in the ODE gives for $\tilde{w} \neq 0$)

$$H_4 k^4 - H_2 k^2 + H_0 = 0 (12)$$

which is a quatric equation in k and can be solved for wavenumbers as

$$k = \pm \sqrt{\frac{H_2 \pm \sqrt{H_2^2 - 4H_4H_0}}{2H_4}}$$
(13)

We can see clearly that the dependence of nonlocal scale parameter $e_0 a$ on wavenumber. These wavenumbers are function of the nonlocal scaling parameter, wave frequency and the material properties of the assumed graphene system.

Computation of Cut-off Frequency: The plot wavenumber vs frequency is called the spectrum curve and in this curve, the frequency at which the imaginary part of wavenumber becomes real is called as cut-off frequency. The cut-off frequencies of flexural wave mode is obtained by setting k = 0 in the dispersion relation (Eq. (12)) i.e., for the present case one can set $H_0 = 0$. The cut-off frequency is obtained as

$$\omega_c^{\text{flexural}} = \sqrt{\frac{C_{22}I_2\eta_m^4}{(J_0 + J_2\eta_m^2)(1 + \mu^2\eta_m^2)} + \frac{K_w + K_G\eta_m^2}{J_0 + J_2\eta_m^2}}$$
(14)

The cut-off frequency is directly proportional to the y-directional wavenumber (η_m) and is also depend on the nonlocal scaling parameter. For $\eta_m = 0$, the wavenumbers of the flexural wave mode have a substantial real part starting from the zero frequency. This implies that the mode starts propagating at any excitation frequency and does not have a cut-off frequency. For $\eta_m \neq 0$, the flexural wave mode, however, has a certain frequency band within which the

corresponding wavenumbers are purely imaginary. Thus, the wave mode does not propagate at frequencies lying within this band. These wavenumbers have a substantial imaginary part along with the real part, thus these waves attenuate as they propagate.

Computation of Escape Frequency: From the spectrum curve, we see that at certain frequency, the flexural wavenumber is tending to infinity and the corresponding wave velocity tends to zero at that frequency. Its value can be analytically determined by looking at the wavenumber expression and setting $k \rightarrow \infty$. This accounts to setting the $H_4 = 0$, which gives

$$\omega_{e}^{flexural} = \frac{1}{\mu} \sqrt{\frac{C_{11}I_{2} + K_{G}\mu^{2}}{J_{2}}}$$
(15)

where ω_e is called escape frequency of the flexural mode.

The phase speed of the wave is defined as $C_p = Real(\omega_n / k)$. Note that the wave speed is also a function of nonlocal scale parameter.

In summary, the plot wavenumber versus frequency is called the spectrum curve and in this curve, the frequency at which the imaginary part of wavenumber becomes real is called as cut-off frequency. The cut-off frequencies of flexural wave mode is obtained by setting k = 0 in the dispersion relation. From the spectrum curve, in nonlocal elasticity calculations, we can see that at certain frequency, the flexural wavenumber is tending to infinity and the corresponding wave velocity tends to zero at that frequency. Such frequency is called as escape frequency. Its value can be analytically determined by looking at the wavenumber expression and setting $k \to \infty$.

III. NUMERICAL EXPERIMENTS, RESULTS AND DISCUSSION

For the present wave propagation analysis, the material properties of the graphene are assumed as: Young's modulus E = 1.06 TPa, thickness h = 0.34 nm, density $\rho = 2300 \text{ kg} / m^3$, and C-C bond length a = 1.42 nm. From literature the values of the polymer matrix Winkler modulus $K_W = 1.13 \times 10^{18}$ Pa/m and polymer matrix shear modulus $K_G = 1.13$ Pa/m are taken from ref. [19].

The flexural wavenumber dispersion with wave frequency in the graphene is shown in Fig. 2, obtained from both local (Figs. 2a and 2b) and nonlocal elasticity (Figs. 2c and 2d) theories, also with and without elastic matrix effect. For the present analysis the nonlocal scaling parameter is assumed as $e_0a = 0$ and 1.0 nm. The spectrum curves shown in figures 2a and 2c are for $\eta_m = 0$ (represents 1D wave propagation), and Figs. 2b and 2d for $\eta_m = 1.0 \text{ nm}^{-1}$ (represents 2D wave propagation). The local elasticity calculation shows that when there is no effect of the elastic matrix, the flexural wavenumber follow a nonlinear variation

at low values of wave frequency; and at higher frequencies it varies linearly as shown in Fig. 2a. This nonlinear variation indicates that the waves are dispersive in nature i.e., the waves will change their shape as they propagate. The linear variation indicates that the waves are in non-dispersive nature, i.e., the wave will not change their shape as they propagate. For $\eta_m = 0$, the wavenumbers of the flexural wave mode have a substantial real part starting from the zero frequency. This implies that the mode starts propagating at any excitation frequency and does not have a cut-off frequency. If we consider the effect of the elastic matrix, initially the flexural wave mode shows a frequency band gap (see Fig. 2a). The frequency band within which the corresponding wavenumbers are purely imaginary. Thus, the flexural mode does not propagate at frequencies lying within this band. So, these wavenumbers have a substantial imaginary part along with the real part, thus these waves attenuate as they propagate. As η_m increases all these waves are still dispersive in nature as shown in Fig. 2b. As the y-directional wavenumber increases from 0 to 1 nm^{-1} , the flexural wave modes are having a frequency band gap region. It has been found that the band gap with matrix effect is greater than the band gap of the without matrix effect (see Fig. 2b). It has also been observed that the frequency band increases with increase in η_m .

The wavenumber dispersion with frequency obtained from nonlocal elasticity ($e_0 a = 1.0 nm$) is shown in Figs. 2c and 2d. The observations made in local elasticity are still valid in nonlocal elasticity also. The only difference is that, because of nonlocal elasticity the wavenumbers of the flexural wave become highly non-linear and tend to infinite at certain frequency. After that frequency the wave will not propagate and the corresponding wave velocities tend to zero at that frequency. This frequency is called as escape frequency or sometimes asymptotic frequency. It can be seen that the wavenumbers before escape frequency are real and after that imaginary. These escape frequencies are not affected by the elastic matrix. Such observation can be clearly seen from Figs. 2c, 2d and Fig. 4b. Here the local/classical elasticity calculation shows that, the wave will propagate even at higher frequencies. But nonlocal elasticity predicts that the waves can propagate up to certain frequencies only, after that it will not propagate (more recently such observations are also made by Narendar and Gopalakrishnan [13, 18] without the elastic matrix effect). Freely standing graphene is always unstable such system can be made stable by resting the graphene on the elastic matrix.

The phase speed dispersions with the wave frequency are shown in Fig. 3, obtained from local and nonlocal elasticity. The observations made in spectrum relations will reflect in the wave speed dispersion curves. Figures 3a and 3b shows that the flexural wave speeds are increasing from low frequency to higher values of wave frequency (local elasticity calculation, $e_0a = 0$). As η_m increases from 0 to 1 nm^{-1} the wave speeds tends to a constant value at higher values of wave frequency. As we move to nonlocality ($e_0 a = 1.0 nm$), the flexural wave stops propagating at certain frequency (i.e.,









Fig. 2 Spectrum curves for a single layer graphene sheet embedded in elastic medium (a) Local elasticity, for $\eta_m = 0$, (b) Local elasticity, for $\eta_m = 1 nm^{-1}$, (c) Nonlocal elasticity ($\mu = e_0 a = 1.0 nm$), for $\eta_m = 0$, and (d) Nonlocal elasticity ($\mu = e_0 a = 1.0 nm$), for $\eta_m = 1 nm^{-1}$.

escape frequency) as shown in Fig. 3c and 3d, this is due to the imaginary part of the wavenumber after the escape frequency. For any value of the η_m , the escape frequency of all flexural waves is same. With and without the elastic matrix effects can also be seen clearly from Fig. 3.

The variation of the cut-off frequency of flexural wave with nonlocal scaling parameter and y-directional wavenumber (η_m) are shown in Figs. 4a and 4b, respectively. The cut-off frequency variation shown in Fig. 3a is for $e_0a = 0, 0.5, 1.0 \text{ and } 2.0 \text{ nm}$. It shows that for a given e_0a , as we increase the y-directional wavenumber the cut-off frequency of flexural wave mode increases. It has been found that at smaller values of the η_m , the cut-off frequencies of the flexural wave will depend on the elastic matrix effect, such difference is clearly seen from Fig. 4a inset. As the nonlocal scaling parameter increases the cut-off frequency decreases. The escape frequency variation with nonlocal scaling parameter is shown in Fig. 4b. It shows that as e0a increases, the escape frequency decreases.

At higher values of e_0a , escape frequencies approach to very small value. For a given nanostructure, nonlocal small scale coefficient can be obtained by matching the results from molecular dynamics (MD) simulations and the nonlocal elasticity calculations. At that value of the nonlocal scale coefficient , the waves will propagate in the nanostructure at that cut-off frequency. In the present paper, different values of e_0a are used. One can get the exact e_0a for a given graphene sheet by matching the MD simulation results of graphene with the results presented in this paper.





(c)

(d)

Fig. 3 Dispersion curves for a single layer graphene sheet embedded in elastic medium (a) Local elasticity, for $\eta_m = 0$, (b) Local elasticity, for $\eta_m = 1 n m^{-1}$, (c) Nonlocal elasticity ($\mu = e_0 a = 1.0 nm$), for $\eta_m = 0$, and (d) Nonlocal elasticity ($\mu = e_0 a = 1.0 nm$), for $\eta_m = 1 n m^{-1}$.

The results are qualitatively different from those obtained based on the local/classical plate theory and thus, are important for the development of GS-based nano-devices such as strain sensor, mass and pressure sensors, atomic dust detectors, enhancer of surface image resolution, etc.





(a)







Fig. 4 Variation of (a) Cut-off and (b) Escape frequencies of the flexural wave in a monolayer graphene sheet embedded in elastic medium.

IV. CONCLUSION

Wave propagation in graphene sheets (GSs) has been a topic of great interest in nanomechanics of GSs, where the equivalent continuum models are widely used. In this manuscript, we examined this issue by incorporating the nonlocal theory into the classical beam model. The influence of the nonlocal effects has been investigated in details. The results are qualitatively different from those obtained based on the local beam theory and thus, are important for the development of GS-based nanodevices such as strain sensor, mass and pressure sensors, atomic dust detectors, enhancer of surface image resolution, etc.

In the present paper, an ultrasonic type of flexural wave propagation nonlocal model is derived for a single layer graphene sheet embedded in elastic matrix. The nonlocal scale parameter introduces certain band gap region in flexural wave mode where no wave propagation occurs. This is manifested in the wavenumber plots as the region where the wavenumber tends to infinite or wave speed tends to zero. It has been shown that the cut-off frequency is a function of nonlocal scaling parameter and the y-directional wavenumber, the escape frequency is purely a function of nonlocal scaling parameter only. Observing the effect of the elastic matrix on the wave dispersion properties of GS is the main theme of this work.

References

- D. Tomanek, R. Enbody, Science and application of nanotubes, Kuwlar/Plenum, NewYork, 2000.
- [2] S. Stankovich, D. Dikin, G. Dommett, K. Kohlhaas, E. Zimney, E. Stach, R. Piner, S. Nguyen, Graphene-based composite materials, *Nature* (London) vol. 442, 2006, pp 282-286.

- [3] P. Sharma, S. Ganti, N. Bhate, Effect of surfaces on the size-dependent elastic state of nano-inhomogeneities. *Applied Physics Letters*, Vol. 82 2003, pp. 535-537.
- [4] C. T. Sun, H. Zhang, Size-dependent elastic moduli of plate like nanomaterials, *Journal of Applied Physics*, Vol. 93, 2003, pp. 1212.
- [5] M. Terrones, N. Grobert, W. Hsu, Y. Hu, J. Terrones, H. Kroto, and D. Ealton, Bulk gass forming metallic alloys: Science and Technology, *Material Research Bulletin*, Vol. 24, 1999, pp. 43-56.
- [6] A.C. Eringen, D.G.B. Edelen, On non-local elasticity. International Journal of Engineering Science, Vol. 10, 1972, pp. 233-245.
- [7] A.C. Eringen, On differential equations of nonlocal elasticity and solutions of screw dislocation and surface waves. *Journal of Applied Physics*, Vol. 54, 1983, pp. 4703-4710.
- [8] J. Peddieson, G. R. Buchanan, and R. P. McNitt, Application of nonlocal continuum models to nanotechnology, *International Journal of Engineering Science*, Vol. 41, 2003, pp. 305-312.
- [9] Y.Q. Zhang, G.R. Liu, X.Y. Xie, Free transverse vibration of doublewalled carbon nanotubes using a theory of nonlocal elasticity. *Physical Review B*, Vol. 71, 2005, pp. 195404.
- [10] C. M. Wang, Y. Y. Zhang, S. S. Ramesh, S. Kitipornchai, Buckling analysis of microand nano-rods/tubes based on nonlocal Timoshenko beam theory. *Journal of Physics D: Applied Physics*, Vol. 39 2006, pp. 3904-3909.
- [11] L. F. Wang, H. Y. Hu, W. L. Guo, Validation of the non-local elastic shell model for studying longitudinal waves in single-walled carbon nanotubes. *Nanotechnology*, Vol. 17, 2006, pp. 1408-1415.
- [12] S. Narendar, S. Gopalakrishnan, Nonlocal scale effects on wave propagation in multi-walled carbon nanotubes, *Computational Materials Science*, Vol. 47, 2009, pp. 526-538.
- [13] S. Narendar, S. Gopalakrishnan, Investigation of The Effect of Nonlocal Scale on Ultrasonic Wave Dispersion Characteristics of a Monolayer Graphene, *Computational Materials Science*, Vol. 49, 2010, pp. 734-742.
- [14] A. N. Cleland, Foundation of nanomechanics, Sringer, 2002.
- [15] M. Born and K. Huang, Dynamical theory of crystal lattices, Clarendon Press, Oxford, 2002.
- [16] S. Gopalakrishnan, A. Chakraborty, D. Roy Mahapatra, Spectral finite element method, Springer Verlag London Ltd., 2008.
- [17] J. F. Doyle, Wave propagation in structures, Springer-VerlagInc, New York, (1997).
- [18] S. Narendar, S. Gopalakrishnan, Strong nonlocalization induced by small scale parameter on Terahertz flexural wave dispersion characteristics of a monolayer grapheme, *Physica E: Low-Dimensional Systems and Nanostructures*, Vol. 43, 2010, pp. 423-430.
- [19] S. C. Pradhan, J. K. Phadikar, Small scale effect on vibration of embedded multilayered graphene sheets based on nonlocal continuum models, *Physics Letters A*, Vol. 373, 2009, pp. 1062-1069

S. Narendar born on March 7, 1986 at Medak District, Andhra Pradesh, India. He received his Bachelor of Technology degree in Aeronautical Engineering from Institute of Aeronautical Engineering, Jawaharlal Nehru Technological University, Hyderabad, India in 2007. He received his Master's degree in Aerospace Engineering in 2009 from Department of Aerospace Engineering, Indian Institute of Science, Bangalore, India. His research interests include: Non-local modelling of 1-D and 2-D nanostructures, stress and strain gradient non-local models, structural dynamics and wave propagation at Terahertz level, spectral finite element analysis, nanocomposites, non-local fluid structure interaction at nanoscale and damage mechanics. Presently, he is working as scientist in Defence Research and Development Laboratory, Kanchanbagh, Hyderabad, India.

S. Gopalakrishnan is currently a professor in the Department of Aerospace Engineering, Indian Institute of Science, Bangalore, India. He obtained his PhD in Aerospace Engineering from Purdue University, W. Lafayette, Indiana, USA. His research interests include Structural Health Monitoring and Smart Structures, Structural Dynamics and Wave Propagation, Modeling and Analysis of MEMS and Nano Structures, Finite Element Analysis, Composites, Fluid-Structure Interaction and Fracture Mechanics. He has published more than 100 international journal papers and two text books on Spectral Finite Element Method and Smart material structures and MEMS.