Vibrational characteristics of single-walled carbon-nanotube: Time and frequency domain analysis

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In this paper, the vibrational characteristics of higher modes of single-walled carbon-nanotube (SWNT) modeled as the continuum axisymmetric cylinder are studied in both time and frequency domains. The modeling of SWNT for the high frequency dynamic analysis is done using the wavelet based spectral element method and this numerical technique involves the Daubechies scaling function approximation in time and one spatial (axial) dimension. This model is capable of capturing the coupled longitudinal-radiation vibration arising due to the finiteness of SWNT. Here, first the phonon dispersion relation is obtained and validated with the atomistic and other continuum model simulations available. The effects of dimensional parameters on higher radial, longitudinal, and coupled radial-longitudinal vibrational modes are studied. Dependence of the higher mode frequencies on these parameters are much different from that of the first mode frequencies. Further time domain responses for broadband excitations are simulated and effects of the radius and thickness of the SWNT are studied. The prominent influence of the above geometrical parameters are observed in the time domain results. © 2007 American Institute of Physics.

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I. INTRODUCTION

Carbon nanotubes (CNTs) have been increasingly attracting a great deal of experimental and theoretical attention since there discovery in 1991. The symmetric structure of CNTs results in extraordinary mechanical properties, such as high specific strength and resilience, together with enormous electrical and thermal conductivities. A recent trend in research shows a growing interest in vibration and wave propagation in CNTs due to their various applications in nanoscale devices, superconductivity, transport, and optical phenomena. Though several atomistic models have been successfully used to obtain the vibrational characteristics of CNTs, the associated computational cost encourages continuum modeling in SWNT and MWNTs.

In Ref. 10 wave propagation in multiwalled carbon nanotubes (MWNTs) were studied considering the Euler-Bernoulli beam theory and was further extended to the Timoshenko beam theory. Wave propagation in MWNTs embedded composites were analyzed in frequency and time domains using the higher order shear deformation beam theory in Ref. 14. Modeling of infinite single-walled carbon-nanotube (SWNTs) through the continuum approach is done to study the acoustic modes and low frequency phonons including the electron-phonon interaction. Continuum elasto-dynamic equations are used to study the low frequency vibration in SWNTs under the infinite length approximation and finite length SWNTs with radial-longitudinal coupling, however, both the studies considered thin wall limits. In Ref. 3, the SWNT wall thickness was incorporated in the continuum model and was fitted to simulate the accurate low frequency phonon dispersion relation. The Flügge equations for continuum modeling were used to study axisymmetric vibrations and wave propagation in SWNT and MWNTs.

In the present work, SWNT is modeled as axisymmetric, finite length, continuum hollow cylinder. The governing elasto-dynamic differential equations for this axisymmetric case consist of two coupled Partial Differential Equation (PDEs) with radial and longitudinal displacements as the variables. These PDEs are solved using a wavelet based spectral element (WSE) method. In this numerical technique, Daubechies scaling function approximation is done in time and in an axial dimension. This reduces the governing PDEs to a set of Ordinary Differential Equation (ODEs) in the radial dimension. The reduced ODEs have variable coefficients and have Bessel’s function solution. The constants involved in Bessel’s function solutions are determined from boundary conditions, i.e., boundary displacements and forces. A similar wavelet based spectral finite element (WSFE) has been developed for wave propagation analysis in isotropic plates, however, unlike the present problem, here the PDEs involved have constant coefficients.

The main advantage of this wavelet based modeling technique is that unlike the Fourier transform based modeling approaches, this technique can efficiently simulate vibrational responses of the finite dimension SWNT. This is primarily due to the localized nature of the Daubechies scaling functions used for the temporal and spatial approximation. In other words, the local support of the basis functions in the WSE method allows the finite domain analysis and imposition of the initial/boundary condition. Thus, finite length structures can be accurately modeled for both the time and frequency domain analysis, and this is not otherwise possible with the prevalent Fourier transform based numerical...
method. This can be attributed to the global support of the bases used in the later method. As a result, it requires periodicity assumption for the temporal approximation and also the assumption of unboundedness in one spatial direction. The consequence of this is that the Fourier transform based numerical methods are mainly restricted to the study of the dispersion relation in the frequency domain and cannot perform the time domain analysis of finite length SWNTs. In summary it can be said that the present method circumvents these limitations and can precisely predict the behavior of finite length SWNTs in both time and frequency domains.

The paper deals with both the frequency and time domain analysis. The frequency domain analysis gives the vibrational and wave characteristics such as the natural frequency, dispersion relation, etc. Such studies help in understanding the physical properties of vibration and wave propagation. However, the time domain analysis helps in visualizing the physical response of the structure due to different excitations. The longitudinal optical modes of SWNTs have been studied using continuum modeling. In Refs. 21, 25 and 26 infinite SWNTs and finite length MWNTs were considered, respectively, to study the pure longitudinal optical modes. However, coupled longitudinal-radial modes were studied in finite length SWNT using continuum approach within thin wall approximation. In all the cases the studies are limited to the analysis of dispersion relations. As stated earlier, the present model has no such restriction and can be used to predict the frequencies of the coupled radial-longitudinal mode occurring due to the finite length of the SWNT.

Here, the proposed WSE method is first used to study the frequencies of radial, longitudinal, and coupled radial-longitudinal modes of a finite length SWNT of different radius and wall thickness. The effects of these geometrical parameters on the higher frequencies of the different vibrational modes are studied. The fundamental radial breathing mode frequencies and the acoustic dispersion relation of SWNT are validated with experimental, atomistic, and continuum modeling results reported in literature. Their dependence on wall thickness and radius are also validated. Next, the wave propagation in the SWNTs due to point impulse load applied in radial/axial directions at the midpoint of the length is studied in the time domain. Even in this case, the effects of radius and wall thickness on the responses are studied. Such analysis of time domain responses are particularly important for sensor applications of CNTs. Simulation and study of these time domain responses are not possible using the Fourier transform based methods widely reported in literature. It should be restated that the present method can perform such analysis due to the localized basis function used for temporal approximation. This is a major advantage of the developed technique over the existing Fourier transform based methods.

II. MATHEMATICAL FORMULATION

A. Governing differential equation

The governing three-dimensional (3D) elasto-dynamic equation for a hollow cylinder is given as

\[ \mu \nabla^2 \mathbf{u} + (\lambda + \mu) \nabla (\nabla \cdot \mathbf{u}) = \rho \partial_t^2 \mathbf{u}, \]

\[ \nabla = (1/r \partial_r r) \mathbf{e}_r + (1/r \partial_{\theta} \theta) \mathbf{e}_\theta + (\partial_z) \mathbf{e}_z, \]  

where \((r, \theta, z)\) is the cylindrical coordinate system and denote radial, circumferential, and axial directions, respectively. \(\mathbf{u} = \{u, v, w\}\) is the displacement vector in radial, circumferential, and axial directions, respectively. \(\lambda, \mu\) are the Lamé's constants. For the axisymmetric condition, the variation with respect to \(\theta\) is not considered. Hence, by considering only radial displacement \(u\) and longitudinal displacement \(w\), Eq. (1) reduces to two coupled PDEs as

\[ (\lambda + 2\mu) \nabla^2 \Delta u + \frac{\partial^2 \Delta}{\partial t^2} \text{ or } c_d^2 \nabla^2 \Delta = \frac{\partial^2 \Delta}{\partial t^2}, \]  

\[ \text{where } c_d^2 = (\lambda + 2\mu)/\rho, \]  

\[ \mu \nabla^2 \Omega_{\theta} = \rho \frac{\partial^2 \Omega_{\theta}}{\partial t^2} \text{ or } c_s^2 \nabla^2 \Omega_{\theta} = \frac{\partial^2 \Omega_{\theta}}{\partial t^2}, \]  

\[ \text{where } c_s^2 = \mu/\rho, \]  

\[ \nabla_n^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{n^2}{r^2} + \frac{\partial^2}{\partial z^2}, \quad n = 0, 1, \]

where the variables \(\Delta\) and \(\Omega_{\theta}\) are defined as

\[ \Delta = \frac{1}{r} \frac{\partial}{\partial r} \left( ru \right) + \frac{\partial w}{\partial z} \]  

\[ \text{and } \Omega_{\theta} = \frac{\partial u}{\partial z} - \frac{\partial v}{\partial r}. \]  

Using Eq. (4), the governing PDEs in terms of displacements can be written in a decoupled form as

\[ \nabla^2 u = \frac{\partial \Delta}{\partial r} + \frac{\partial \Omega_{\theta}}{\partial z}, \]

\[ \nabla^2 w = \frac{\partial \Delta}{\partial z} - \frac{1}{r} \frac{\partial (ru)}{\partial r}. \]  

The associated boundary conditions are given as

\[ \sigma_r = \lambda \Delta + 2 \mu \frac{\partial u}{\partial r}, \]

\[ \sigma_z = \mu \frac{\partial u}{\partial z} + \frac{\partial w}{\partial r}, \]

where \(\sigma_r\) and \(\sigma_z\) are the radial and axial forces, respectively, acting on the surface of the cylinder along the \(z\) direction.

B. Daubechies compactly supported wavelets

A concise review of the orthogonal basis of Daubechies wavelets is provided. Wavelets, \(\psi_{j,k}(t)\) forms compactly supported orthonormal basis for \(L^2(\mathbb{R})\). The wavelets and the associated scaling functions \(\varphi_{j,k}(t)\) are obtained by translation and dilation of single functions \(\varphi(t)\) and \(\varphi(t)\), respectively

\[ \psi_{j,k}(t) = 2^{j/2} \varphi(2^j t - k), \quad j, k \in \mathbb{Z}, \]
\[ \varphi_{j,k}(t) = 2^{j/2} \varphi(2^j t - k), \quad j, k \in \mathbb{Z}. \]  

The scaling functions \( \varphi(t) \) are derived from the dilation or scaling equation

\[ \varphi(t) = \sum_k a_k \varphi(2t - k), \quad (11) \]

and the wavelet function \( \psi(t) \) is obtained as

\[ \psi(t) = \sum_k (-1)^k a_{1-k} \varphi(2t - k), \quad (12) \]

\( a_k \) are the filter coefficients and they are fixed for specific wavelet or scaling function basis. For compactly supported wavelets only a finite number of \( a_k \) are nonzero. The filter coefficients \( a_k \) are derived by imposing certain constraints on the scaling functions which are as follows. (1) The area under scaling function is normalized to one; (2) the scaling function \( \varphi(t) \) and its translates are orthonormal; and (3) the wavelet function \( \psi(t) \) has \( M \) vanishing moments. The number of vanishing moments \( M \) denotes the order \( N \) of the Daubechies wavelet, where \( N = 2M \).

Let \( P_j(f)(t) \) be the approximation of a function \( f(t) \) in \( L^2(\mathbb{R}) \) using \( \varphi_{j,k}(t) \) as basis, at a certain level (resolution) \( j \), then

\[ P_j(f)(t) = \sum_k c_{j,k} \varphi_{j,k}(t), \quad k \in \mathbb{Z}, \quad (13) \]

where \( c_{j,k} \) are the approximation coefficients.

**C. Temporal approximation using Daubechies scaling functions**

The first step in the formulation of WSE is the reduction of each of the two governing differential equations given by Eqs. (2) and (3) with variables \( \Delta \) and \( \Omega_n \) to a set of PDEs in the spatial dimensions by the Daubechies scaling function based transformation in time. The procedure is very similar to the wavelet based spectral finite element formulation for isotropic plates discussed earlier in Ref. 24. Let \( \Delta(r,z,t) \) be discretized at \( n \) points in the time window \( [0,t_f] \). Let \( t = 0,1,\ldots,n-1 \) be the sampling points then

\[ t = \Delta t, \quad (14) \]

where \( \Delta t \) is the time interval between two sampling points. The function \( \Delta(r,z,t) \) can be approximated by scaling function \( \varphi(\tau) \) at an arbitrary scale as

\[ \Delta(r,z,t) = \sum_k \Delta_k(r,z) \varphi(\tau - k), \quad k \in \mathbb{Z}, \quad (15) \]

where \( \Delta_k(r,z) \) (referred as \( \hat{\Delta}_k \) hereafter) are the approximation coefficient at a certain spatial dimension \( r \) and \( z \) and Eq. (2) can be written as

\[ \sum_k c^2 \left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} \right] \Delta_k \varphi(\tau - k) = \Delta^2 \sum_k \Delta_k \varphi^\prime(\tau - k). \quad (16) \]

Taking the inner product on both sides of Eq. (16) with the translates of scaling functions \( \varphi(\tau - j) \), where \( j = 0,1,\ldots,n - 1 \) and using their orthogonal properties, we get \( n \) simultaneous PDEs as

\[ c^2 \left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} \right] \Delta_j = \Delta^2 \sum_{k=0}^{n-2} \Omega^2_{j-k} \Delta_k, \quad j = 0,1,\ldots,n-1, \quad (17) \]

where \( N \) is the order of the Daubechies wavelet and \( \Omega^2_{j-k} \) are the second-order connection coefficients. The \( p \)-th order connection coefficients are defined as

\[ \Omega^p_{j-k} = \int \varphi^p(\tau - k) \varphi(\tau - j) d\tau. \quad (18) \]

For compactly supported wavelets, \( \Omega^2_{j-k} \) are nonzero only in the interval \( k = j-N+2 \) to \( k = j+N-2 \). The details for evaluation of connection coefficients for different orders of derivative is given by Beylkin.31

It can be observed from the PDEs given by Eq. (17) that certain coefficients \( \Delta_j \) near the vicinity of the boundaries \( j = 0 \) and \( j = n-1 \) lie outside the time window \( [0,t_f] \) defined by \( j = 0,1,\ldots,n-1 \). These coefficients must be treated properly for the finite domain analysis. Here, a wavelet based extrapolation scheme32 is implemented which uses polynomial extrapolation the coefficients lying outside the finite domain either from interior coefficients or initial/boundary values. The method is particularly suitable for approximation in time for the ease to impose initial values. The above method converts the PDEs given by Eq. (17) to a set of coupled PDEs given as

\[ \sum_k c^2 \left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} \right] \{ \Delta_j \} = \{ \Gamma^1 \} \{ \Delta_j \}, \quad (19) \]

where \( \Lambda^1 \) is the first-order connection coefficient matrix obtained after using the wavelet extrapolation technique. These coupled PDEs are decoupled using eigenvalue analysis

\[ \Gamma^1 = \Phi \Lambda \Phi^{-1}, \quad (20) \]

where \( \Pi \) is the diagonal eigenvalue matrix and \( \Phi \) is the eigenvectors matrix of \( \Gamma^1 \). Let the eigenvalues be \( \gamma_j, \lambda = \sqrt{-1} \), then the decoupled PDEs corresponding to Eq. (19) are

\[ c^2 \left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} \right] \hat{\Delta}_j = - \gamma^2_j \hat{\Delta}_j, \quad j = 0,1,\ldots,n-1, \quad (21) \]

where \( \hat{\Delta}_j \) is

\[ \hat{\Delta}_j = \Phi^{-1} \Delta_j. \quad (22) \]

Following the same steps, the final transformed form of Eq. (3) is

\[ c^2 \left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{1}{r^2} + \frac{\partial^2}{\partial z^2} \right] \hat{\phi}_{j,0} = - \gamma^2_j \hat{\phi}_{j,0}, \quad j = 0,1,\ldots,n-1. \quad (23) \]

Similarly, the transformed form of the decoupled displacement equations [Eqs. (5) and (6)] and force boundary conditions [Eqs. (7) and (8)] can be written as

\[ \varphi_{j,k}(t) = 2^{j/2} \varphi(2^j t - k), \quad j, k \in \mathbb{Z}. \]
\begin{equation}
\nabla^2 \hat{u}_j = \frac{\partial \bar{\Delta}_j}{\partial r} + \frac{\partial ^2 \bar{\Delta}_j}{\partial z^2}, \quad \nabla^2 \hat{w}_j = \frac{\partial \bar{\Delta}_j}{\partial z} - \frac{1}{r} \left( \frac{\partial (r \bar{\Delta}_j)}{\partial r} \right),
\end{equation}

\begin{equation}
\bar{\sigma}_{ij} = \lambda \bar{\Delta}_{ij} + 2 \mu \frac{\partial \hat{u}_j}{\partial r}, \quad \bar{\sigma}_{ij} = \mu \frac{\partial \hat{u}_j}{\partial z} + \frac{\partial \hat{w}_j}{\partial r},
\end{equation}

where \( \bar{\sigma}_{ij} \) and \( \bar{\sigma}_{ij} \) are the transformed forces \( \sigma_r(r,z,t) \) and \( \sigma_z(r,z,t) \), respectively.

**D. Spatial approximation using Daubechies scaling functions**

As stated earlier, the next step involved is to further reduce each of the transformed and decoupled PDEs given by Eqs. (21) and (23) for \( j=0,1, \ldots, n-1 \) to a set of coupled ODEs using Daubechies scaling function approximation in one of the axial (Z) direction. Similar to time approximation, the transformed variable \( \hat{\Delta}_j \) is discretized at \( m \) points in the spatial window \([0, L_z]\), where \( L_z \) is the length in the z direction. Let \( \xi = 0,1, \ldots, m-1 \) be the sampling points, then

\[ z = \Delta z \xi, \]

where \( \Delta z \) is the spatial interval between two sampling points. The function \( \hat{\Delta}(r, \xi) \) can be approximated by scaling function \( \varphi(\xi) \) at an arbitrary scale as

\[ \hat{\Delta}(r, \xi) = \sum_k \hat{\Delta}(r) \varphi(\xi - l), \quad l \in \mathbb{Z}, \]

where \( \hat{\Delta}(r, \xi) \) (referred to as \( \hat{\Delta}_j \) hereafter) is the approximation coefficient at a certain radial dimension \( r \). Thus Eq. (21) can be written as

\[ c^2 \left[ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right] \Delta_j \varphi(\xi - l) + c^2 \frac{1}{\Delta_z^2} \Delta_j \varphi''(\xi - l) = -\gamma^2 \Delta_j \varphi(\xi - l). \]

Taking the inner product on both sides of Eq. (28) with the translates of scaling functions \( \varphi(\xi - l) \), where \( l = 0,1, \ldots, m-1 \) and using their orthogonal properties, we get \( m \) simultaneous ODEs as

\[ c^2 \left[ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right] \Delta_j + c^2 \frac{1}{\Delta_z^2} \sum_{i=-n+2}^{i=N-2} \Delta_j \Omega^{ij} = -\gamma^2 \Delta_j, \]

\[ i = 0,1, \ldots, m-1, \]

where \( \Delta \) is the order of Daubechies wavelet, \( \Omega^{ij} \) is the connection coefficients for the second-order derivative defined in Eq. (18).

Even here certain coefficients lying outside the finite domain given by \([0, L_z]\), must be treated properly for the finite domain analysis. However, unlike the time approximation, these coefficients are obtained through the periodic extension. Here, after expressing the unknown coefficients lying outside the finite domain in terms of the inner coefficients considering periodic extension, the ODEs given by Eq. (29) can be written as a matrix equation of the form

\[ c^2 \left[ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right] \Delta_j + c^2 \sum_{i=1}^{m} \Delta_j \Lambda^{ij} = -\gamma^2 \Delta_j, \]

where \( \Lambda^{ij} \) is the first-order connection coefficient matrix obtained after periodic extension and has a circulant form.

The coupled ODEs given by Eq. (30) are decoupled using eigenvalue analysis similar to that completed in the time approximation as

\[ \Lambda = \Psi \Psi^{-1}, \]

where \( \Psi \) is the diagonal eigenvalue matrix and \( \Psi \) is the eigenvectors matrix of \( \Lambda \). It should be mentioned here that for a circulant matrix \( \Lambda \), eigenparameters are known analytically.\(^{33}\) Let the eigenvalues be \( \imath \beta_i \), then the decoupled ODEs corresponding to Eq. (30) are

\[ c^2 \left[ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \beta_i \right] \Delta_{ij} = -\gamma^2 \Delta_{ij}, \quad i = 0,1, \ldots, m-1, \]

where \( \Delta_{ij} \) is

\[ \Delta_{ij} = \Psi^{-1} \Delta_{ij}. \]

Following similar steps, the final transformed form of Eq. (23) is given by

\[ c^2 \left[ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \beta_i \right] \Omega_{ij} = -\gamma^2 \Omega_{ij}. \]

Similarly the decoupled displacement Eqs. (24) and (25) can be written as

\[ \left[ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \beta_i \right] \tilde{u}_{ij} = \imath \beta \tilde{\Omega}_{ij}, \]

\[ \left[ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \beta_i \right] \tilde{w}_{ij} = -\imath \beta \tilde{\Delta}_{ij} - \frac{1}{r} \frac{d}{dr} \left( r \tilde{\Omega}_{ij} \right), \]

\[ \tilde{\sigma}_{ij} = \lambda \tilde{\Delta}_{ij} + 2 \mu \tilde{u}_{ij}, \]

\[ \tilde{\sigma}_{ij} = -\imath \beta \mu \tilde{u}_{ij} + \frac{d \tilde{w}_{ij}}{dr}. \]

These transformed and decoupled ODEs given by Eqs. (32) and (34) and (35)–(38) are solved using Bessel’s functions described in the next subsection.

**E. Bessel’s function solutions**

Here, Bessel’s functions are used for the solution of the transformed governing equation given by Eqs. (32) and (34). The solutions for \( \tilde{\Delta} \) and \( \tilde{\Omega} \) are obtained as

\[ \tilde{\Delta}(r) = C_1 J_0(\imath \beta r) + C_2 Y_0(\imath \beta r), \]

where \( J_0 \) and \( Y_0 \) are Bessel’s functions of the first and second kind of order zero, respectively.
\[ \tilde{\nu}(r) = C_2 J_1(k r) + C_4 Y_1(k r), \]  
(40)

where \( k^2 = (\rho' / c_p^2 - \beta^2) \), \( k_0^2 = (\rho' / c_s^2 - \beta^2) \), and \( C_1, C_2, C_3, C_4 \) are constants. \( J_n \) and \( Y_n \) are Bessel’s functions of the first and second kind.

Substituting Eqs. (39) and (40) into Eqs. (35) and (36) and solving for \( \tilde{u} \) and \( \tilde{w} \) gives

\[ \tilde{u}(r) = -k_2 \left[ C_1 J_1(k r) + C_2 Y_1(k r) \right] , \]
\[ -i \beta \left[ C_1 J_1(k r) + C_4 Y_1(k r) \right] , \]
\[ \tilde{w}(r) = -1 \beta \left[ C_1 J_0(k r) + C_2 Y_0(k r) \right] \]
\[ -k_3 \left[ C_1 J_0(k r) + C_4 Y_0(k r) \right] . \]
(41)

(42)

The above solutions provide the interpolating functions for forming the elemental dynamic stiffness matrix. The unknown constants \( \{a\} = \{C_1, C_2, C_3, C_4\} \) can be determined from the transformed nodal displacements \( \tilde{u}(r), \tilde{w}(r) \) at inner \( (r = r_i) \) and outer \( (r = r_o) \) radii. The nodal displacement vector is \( \{\tilde{u}\} = [\tilde{u}_1, \tilde{u}_2, \tilde{w}_1, \tilde{w}_2] \), where \( \tilde{u}_1 = \tilde{u}(r_i), \tilde{w}_1 = \tilde{w}(r_i) \), \( \tilde{u}_2 = \tilde{u}(r_o) \), and \( \tilde{w}_2 = \tilde{w}(r_o) \). Thus we can relate nodal displacements and unknown constants from Eqs. (41) and (42) as

\[ \{\tilde{u}\} = [B] \{a\} . \]
(43)

Substituting Eqs. (41) and (42) in the transformed boundary conditions Eqs. (37) and (38), they can be written as

\[ \tilde{\sigma}_r(r) = \left[ -\{\lambda + 2 \mu k_2^2 - \lambda \beta^2\} J_0(k r) \right. \]
\[ + 2 \mu k_2^2 J_1(k r) J_0(k r) \left[ C_1 + \left\{\lambda + 2 \mu k_2^2 - \lambda \beta^2\right\} Y_0(k r) \right] \]
\[ + 2 \mu k_2^2 Y_1(k r) J_0(k r) \left[ C_2 + \left\{\lambda + 2 \mu k_2^2 - \lambda \beta^2\right\} Y_1(k r) \right] \]
\[ + 2 \mu k_2^2 \beta^2 \left[ J_0(k r) - J_1(k r) \right] \left[ C_3 + \left\{\lambda + 2 \mu k_2^2 - \lambda \beta^2\right\} Y_0(k r) \right] \]
\[ + 2 \mu k_2^2 \beta^2 \left[ J_1(k r) - J_0(k r) \right] \left[ C_4 + \left\{\lambda + 2 \mu k_2^2 - \lambda \beta^2\right\} Y_1(k r) \right] \],
(44)

\[ \tilde{\sigma}_z(r) = -2 \mu \beta k_2 \left[ J_1(k r) C_1 + Y_1(k r) C_2 \right] \]
\[ - \mu (k_2^2 - \beta^2) \left[ J_1(k r) C_3 + Y_1(k r) C_4 \right] , \]
(45)

From the two above equations, the nodal force vector \( \{F^r\} = \{\tilde{\sigma}_r, \tilde{\sigma}_z, \tilde{\sigma}_{r2}, \tilde{\sigma}_{z2}\} \) can be related to the constants \( \{a\} \) as

\[ \{F^r\} = [C] [a] . \]
(46)

where \( \tilde{\sigma}_{r1} = \tilde{\sigma}_r(r_i), \tilde{\sigma}_{z1} = \tilde{\sigma}_z(r_i), \tilde{\sigma}_{r2} = \tilde{\sigma}_r(r_o), \) and \( \tilde{\sigma}_{z2} = \tilde{\sigma}_z(r_o) \). Finally from Eqs. (43) and (46), a relation between transformed nodal forces and displacements is obtained as

\[ \{F^r\} = \left[ C \right] [B]^{-1} \{\tilde{u}\} = \left[ K^r \right] \{\tilde{u}\} , \]
(47)

where \( [K^r] \) is the exact elemental dynamic stiffness matrix. Thus solving Eq. (47) for transformed displacement vector \( \{\tilde{u}\} \) from the transformed load vector \( \{F^r\} \), the actual displacements are obtained by performing an inverse wavelet transform twice for time and spatial dimension.

III. NUMERICAL EXPERIMENTS

A. Frequency domain analysis

In this work numerical experiments are performed to study the effect of thickness, \( 2h \) and radius, \( R \) of the SWNT on the higher axisymmetric vibrational modes. The vibration includes predominantly radial breathing modes (RBMs) and longitudinal modes, and coupled radial-longitudinal modes. Here the uncoupled pure twisting mode resulting from circumferential displacement is not considered. The bulk material properties are, Young’s modulus \( E_h = 360 \text{ J/m}^2 \), mass density \( \rho_h = 2270 \times 0.34 \text{ kg/m}^3 \), and Poisson’s ratio \( v = 0.2 \).

In particular these parameters are not dependent on the definition of thickness \( 2h \). The variation of Young’s modulus with radius is not well defined. In Ref. 36 it has been stated that Young’s modulus does not vary with the radius, while the variation has been predicted in Refs. 9 and 37. Considering uniform Young’s modulus irrespective of the radius varying between 0.3 and 1.0 nm, the fundamental RBM frequencies are found to follow the \( \frac{1}{2} R \) law in tune with the experimental results. Thus in this work, the Young’s modulus is considered to be independent of the radius. The radius \( R \) of \( (N, N) \) SWNT is calculated as \( R = 3Na_{C-C}/(2 \pi) \), where \( a_{C-C} \) is carbon bond length and equal to 0.142 nm. The inner and outer radius are referred as \( a = R - h \) and \( b = R + h \), respectively. The frequencies are expressed in optical units cm\(^{-1}\), where the conversion is given as 1 Hz = 3.336 \times 10^{11} \text{ cm}^{-1}.

As mentioned earlier, the developed SWNT model is validated by comparing the simulated results with those available in literature. In Fig. 1, the acoustic phonon dispersion relation of a (10,10) SWNT with \( R = 0.678 \text{ nm} \) and \( 2h = 0.09 \text{ nm} \) are presented for the axisymmetric condition. Comparisons are made with the corresponding results \( n = 0 \) obtained from \textit{ab initio} and 3D elasto-dynamic continuum models. In the figure, the frequencies in optical units are presented for varying longitudinal wavenumber \( K_z \), normalized as \( K_z/\alpha \). In the present formulation \( K_z \) represent \( \beta \).
as in Eq. (32). Similar to Refs. 3 and 4 the dispersion relation is obtained by equating the determinant of the matrix [C] in Eq. (46) to zero and solving for \( \gamma \) for different values of \( \beta \), i.e., \( K \). Though the radial and longitudinal displacements are only considered in this work, here, the axisymmetric circumferential displacement is also studied and compared. It can be seen that the acoustic phonon dispersion relation predicted by the present model is in good agreement with that obtained from Ref. 3 and 8.

Next, the higher axisymmetric vibrational modes are studied to understand the effect of geometrical parameters on these higher natural frequencies. Figure 2(a) shows the variation of the first two RBMs with \( 2h \) for a SWNT of \( R = 0.678 \text{ nm} \) and length \( L = 25 \text{ nm} \). The wall thickness is varied from \( 2h = 0.24 - 0.34 \text{ nm} \). It can be seen that the first frequency of RBM is not dependent on the SWNT wall thickness considered in the continuum model. This is in tune with that stated in Ref. 3 and other theoretical work.4,35 The first RBM frequency calculated is 179 cm\(^{-1}\) which compares well with the value 182 cm\(^{-1}\) derived in Ref. 3 and is close to the experimental value,186 cm\(^{-1}\). A better match between the results can be obtained by fitting the bulk material properties such as Young’s modulus, mass density, and Poisson’s ratio. However, interestingly, it has been observed that the higher RBM frequencies vary considerably with the SWNT wall thickness. One explanation for this behavior is that at higher RBM modes, the deformation varies along the thickness of the SWNT. In other words, at higher frequencies, local deformation of the SWNT wall occurs along with the overall radial breathing deformation. This makes the higher RBM frequencies dependent on the wall thickness. Apart from this, at higher frequencies the effect of radial-longitudinal coupling is more prominent which may also be a reason for such behavior. As described earlier, these coupling effects can only be captured by the present modeling technique which takes into account the finiteness of the structure. However, this observation is of much importance as it suggests that in continuum modeling the wall thickness has to be fitted from the experimental results to correctly predict the higher RBM frequencies unlike the first RBM frequency.

In Fig. 2(b), the first two RBM frequencies of SWNT are plotted for varying radius \( R \) from 0.3 to 1.0 nm. The length of SWNT is \( L = 25 \text{ nm} \) and \( 2h = 0.34 \text{ nm} \). It can be seen that the variation of first RBM frequency is linear and obeys the \( 1/d \) rule. This has been predicted in Ref. 7. Here, the variation of the first RBM frequency is obtained as 243 cm\(^{-1}\) (nm/2R) which compares well with the value 246 cm\(^{-1}\) (nm/2R) obtained in Ref. 3. Even here, the higher RBM frequencies show a counterintuitive behavior. These frequencies do not vary significantly with the increase in the \( R \) as seen from the figure. Again the complicated nature of the higher frequencies due to the local deformation of SWNT wall and increased effect of longitudinal-radial mode coupling may be an explanation of this behavior.

However, it should be mentioned here that the characteristics of higher RBM frequencies have been studied within a certain region of \( 2h \) and \( R \). Though in this work the viable ranges of \( 2h \) and \( R \) have been considered, it is probable that the trend may vary over other range of these parameters. Furthermore, it has been observed by performing numerical experiments that for a given \( R \), the length \( L \) of SWNT has no significant effect on these frequencies except for very low slenderness (\( L/R \)) ratio which is not common in carbon nanotubes.

Figure 3(a) show the frequencies of the first two longitudinal vibrational modes of a SWNT with \( L = 25 \text{ nm} \), \( R = 0.678 \text{ nm} \), and \( 2h \) varied over 0.24–0.34 nm. It can be seen that both the frequencies have a linear variation with the wall thickness. Such variation is much justified as the longitudinal stiffness and thus the corresponding frequency is primarily dependent on the wall thickness. The slope of the plots are nearly equal for both the modes. The rate of decrease of the longitudinal frequencies with the increase of \( 2h \) is high and hence only a small range is considered for the study. In addition, the frequencies of the longitudinal modes are much higher than the corresponding radial modes. As an example for (10,10) SWNT with \( R = 0.678 \text{ nm} \) and \( 2h = 0.34 \text{ nm} \), the frequency of fundamental longitudinal mode is 692 cm\(^{-1}\) while that of fundamental RBM is 179 cm\(^{-1}\). Thus for determining the longitudinal vibrational frequencies using continuum model, the wall thickness plays an important role.
even for the first mode. Hence, this parameter should also be fitted with the experimental results. In Fig. 3, the first two longitudinal mode frequencies of the SWNT with $L=25$ nm and $2h=0.34$ nm are plotted for different $R$. It is observed that these frequencies are not influenced by the $R$. Similar to the RBMs, even here the length has no effect on the frequencies of longitudinal mode for $L/R < 10$.

The frequencies of radial and longitudinal modes presented in the last two examples though has the effect of the radial-longitudinal coupling particularly at the higher mode, they are predominantly radial or longitudinal modes. However, there exists a mode which results purely from the coupling as also been reported in literature and this causes the coupled vibration, i.e., a radial vibration to occur due to purely axial excitation and vice versa. Again it should be mentioned that these coupled mode frequencies can be obtained using the present wavelet based model unlike Fourier transform based method which assume infinite length SWNT. In Fig. 4(a), the dependence of the first three frequencies of this coupled mode $2h$ are shown for a SWNT with $R=0.678$ nm and $L=25$ nm. The wall thickness are varied from $2h=0.24$ to 0.34 nm. It can be seen that the behavior of these frequencies with varying $2h=0.3−0.5$. Even here, the first frequency is invariant to $2h$, while the other two higher frequencies have linear variation. The frequency of the first coupled mode is very near to the first RBM frequency while the other higher modal frequencies varies considerably. Figure 4(b) shows the frequencies of radial-longitudinal coupled mode of a SWNT with $2h=0.34$ nm and $L=25$ nm for varying $R$ from 0.3 to 1.0 nm. Again here, the trend of variation is similar to that of the RBM frequencies. This coupled vibrational modes are also independent of $L$ for a slenderness ratio $L/R < 10$.

### B. Time domain analysis

The time domain analysis of responses of carbon nanotubes to excitation signals has a wide scope and applications in sensor development. Unlike the Fourier transform based analysis, the present wavelet based formulation allows accurate simulations of time domain responses along with the frequency domain analysis provided earlier. This is due to
the outer surface, the geometrical parameters of SWNT have a prominent influence on the time domain response. This is evidenced through numerical experiments, which show that all time domain responses to a great extent. This has been observed that changing the wall thickness from $2h=0.34$ nm to $2h=0.09$ nm for a SWNT, the vibration pattern changes considerably, though it has been observed from the study of RBM frequencies earlier [see Fig. 2(a)] that the frequencies of only higher RBMs are affected by the parameters $2h$. This may be again justified by the explanation given in the last paragraph. Similar difference in the wave transmission snapshots are observed when the radius of SWNT is increased from $R=0.339$ to 0.475 nm. This difference may have resulted from the effect of $R$ on the first RBM frequency [see Fig. 2(b)]. In Fig. 6, similar snapshots of radial wave propagation at instances $T_1=0.5$ ps and $T_2=1.0$ ps are presented, except that these radial wave propagation results due to the impulse load applied in axial direction at the midpoint of SWNT and at $r=b$. It can be summarized that the wall thickness of SWNT should be fitted from correlation with experimental results to predict the accurate time domain response both radial and longitudinal.

**IV. CONCLUSIONS**

In this work, a wavelet based axisymmetric continuum model of single-walled carbon nanotube is presented. The model allows both time and frequency domain analysis and has been validated with theoretical and experimental results available in literature. The validation is done for the fundamental radial breathing mode and axisymmetric acoustic phonon dispersion relation. The present study mainly focuses on the characteristics and the effect of geometrical parameters on the frequencies of higher radial, longitudinal, and radial-longitudinal vibrational modes. It has been observed that the frequencies of higher radial modes have a linear dependency on the parameters.
variation with the wall thickness while they are invariant to the radius and this is reverse of the behavior exhibited by fundamental radial breathing mode. This behavior of higher radial mode frequencies can be explained as the effect of local deformation of the nanotube wall and the predominant effect of radial-longitudinal coupling. Thus, the wall thickness is an important parameter in continuum modeling to predict higher frequencies. For similar reasons, the continuum model should account for radial-longitudinal coupling for accurate determination of these frequencies. In addition, quite contrary to the fundamental radial breathing mode, the fundamental and higher longitudinal frequencies vary linearly with the wall thickness and is not dependent on the radius. However, the frequencies of the coupled radial-longitudinal vibrational modes show similar pattern of dependence on the radius and wall thickness as shown by the frequencies of radial mode. These coupled radial-longitudinal coupling arises in finite length SWNT and unlike the present method, the simpler Fourier transform based technique cannot predict these modes due to its incapability to model finite length SWNT. Apart from this high frequency analysis, one main advantage of the developed model is that it can be efficiently used for time domain analysis. The response to impulse loading has a significant influence on the wall thickness and radius of the nanotube due to the participation of the higher modes.