Shell element based model for wave propagation analysis in multi-wall carbon nanotubes

A. Chakraborty *

India Science Lab, GM Technical Centre (I), Bangalore 560066, India

Received 19 September 2005; received in revised form 5 May 2006
Available online 6 July 2006

Abstract

A spectrally formulated finite element is developed to study very high frequency elastic waves in carbon nanotubes (CNTs). A multi-walled nanotube (MWNT) is modelled as an assemblage of shell elements connected throughout their length by distributed springs, whose stiffness is governed by the van der Waals force acting between the nanotubes. The spectral element is formulated using the recently developed strategy based on singular value decomposition (SVD) and polynomial eigenvalue problem (PEP). The element can model a MWNT with any number of walls. Studies are carried out to investigate the effect of the number of walls on the spectrum and dispersion relation. The importance of shell element based model over the beam model is established. The zone of validity of the previously developed beam model is also investigated. It is shown that the shell model is required to capture the symmetric Lamb wave modes. It is also shown through numerical examples that the developed element efficiently captures the response of MWNT for Tera-hertz level frequency loading.
© 2006 Elsevier Ltd. All rights reserved.

Keywords: Multi-wall CNT; Wave propagation; Spectral finite element; Shell model; Polynomial eigenvalue problem

1. Introduction

Since their discovery in 1991, CNTs are currently occupying the center-stage of theoretical and experimental attention (Tomanek and Enbody, 2000). It is well-known that by virtue of their special symmetric structures, CNTs possess extraordinary mechanical properties, such as extremely high specific strength, specific stiffness, resilience and enormous electrical and thermal conductivities (Tersoff and Ruoff, 1994; Yakobson et al., 1996a; Treacy et al., 1996; Halicioglu, 1998; Harris, 1999; Govindjee and Sackman, 1999; Yoon et al., 2003). However, to translate these excellent properties to the realm of mechanical applications, it is necessary to have the fundamental understanding of the nanostructured materials. This calls for a good modelling strategy for the CNTs, which should retain the important aspects of the structure without being computationally too expensive.
An extensive account of the theoretical modelling aspects of CNTs, both atomistic and continuum approaches can be found in (Chakraborty et al., 2006), where Euler–Bernoulli (EB) beam theory based spectral finite element (SFE) was developed for MWNTs. Recently, a non-linear analysis is performed using the EB theory to investigate the effect of tube diameter on the bending modulus (Wang et al., 2005). Effect of internal moving fluid on vibration and structural instability is also studied using the EB theory (Yoon et al., 2005). Similar studies are also conducted by Wang and Varadan (2006) to investigate the effect of EB theory and Timoshenko beam theory on the modelling of single and multi-wall nanotubes.

In the present study, a new spectral element based on shell theory is developed. There are few earlier works on the shell-theory based model of CNTs. Yakobson et al. (1996a,b) noticed the unique features of fullerenes and developed a continuum shell model, where the analytical expressions for the energy of a shell in terms of local stresses and deformations were provided. Ru (2000a,b) followed this continuum shell model to investigate buckling of CNTs subjected to axial compression. This kind of continuum shell models can be used to analyze the static or dynamic mechanical properties of nanotubes. However, these models neglect the detailed characteristics of nanotube chirality, and are unable to account for forces acting on the individual atoms.

Spectral finite element method (SFEM) (Doyle, 1997) is arguably the most suitable technique for studying wave propagation in structural waveguides and especially in MWNT due to high frequency content loading (THz level). The basic SFEM is further improved by Chakraborty and Gopalakrishnan where the problem is cast as PEP (Lancaster, 1969) and SVD method of wave amplitude extraction is utilized. This approach puts SFEM in a solid ground and gives it the most generalized form to handle any kind of structure. This method is so far utilized in plate element formulation (Chakraborty and Gopalakrishnan, 2005) and beam approximation of MWNT (Chakraborty et al., 2006).

In the present work, plane strain shell model based SFE is considered for modelling MWNT. Wave numbers and group speeds are determined as functions of the number of walls, which facilitate to get deep insight in the wave propagation response of MWNTs. The present element formulation exploits the PEP method extensively, which is most suitable in the present case as number of walls has been taken as a parameter in element formulation. The organization of the paper is as follows. In Section 2, the details of the element formulation is presented. General methods are also presented to obtain the expressions of cut-off frequencies, spectrum relation and dispersion relation. Section 3 discusses the effect of number of walls on the spectrum and dispersion relation and the wave propagation response due to applied tip shear loading.

2. Mathematical formulation

The present MWNT model is based on the kinematics of shell in plane strain condition. Assuming that the shell has a much larger dimension in the Z-direction compared to the other dimensions in the X–Y-plane (see Fig. 1) and there is no variation in geometry or loading along the Z-direction, the displacement field is assumed as

\[ \bar{u}(s, r, z) = u(s) - r(w_s + R^{-1}u), \quad \bar{v}(s, r, z) = 0, \quad \bar{w}(s, r, z) = w(s), \]

where \( \bar{u}, \bar{v} \) and \( \bar{w} \) are the components in the circumferential \( s = R\theta \), axial \( Z \) and radial direction \( r \), respectively, and the subscript denotes differentiation with respect to \( s \). Here, \( R \) represents the mean radius of the shell.

The non-zero strain and stress corresponding to this displacement field are

\[ \varepsilon_{ss} = -R^{-1}w + u_s - r(w_{ss} + R^{-1}u_s), \quad \sigma_{ss} = \frac{E}{(1 - \nu^2)} \varepsilon_{ss}, \]

where \( E \) and \( \nu \) are the Young’s modulus and Poisson’s ration of the shell material, respectively. Based on the displacement field in Eq. (1), the shell kinetic energy, \( K \) becomes

\[ K = \frac{1}{2} \int_{\theta_1}^{\theta_2} \int_{r_1}^{r_2} \rho(\bar{u}^2 + \bar{w}^2) \, dr \, d\theta, \]
where \( q \) is the density of the material and a dot over a variable denotes differentiation with respect to time. The limits of the integral denote the boundary of the shell in the \( X-Y \)-plane. Similarly, the potential energy, \( P \) is defined as

\[
P = \frac{1}{2} \int_{\theta_1}^{\theta_2} \int_{r_1}^{r_2} \sigma_{ss} \epsilon_{ss} \, dr \, d\theta.
\]

These expressions can be further simplified by integrating in the thickness (\( r \)) direction and noting that the material distribution is symmetric about the mid-plane, i.e., \( \int r \, dr = 0 \).

The governing equations and the boundary conditions are now derived by applying the Hamilton’s principle (minimizing the action integral)

\[
\delta \int_{t_1}^{t_2} H \, dt = \delta \int_{t_1}^{t_2} (K - P) \, dt = 0,
\]

which yields the governing equations

\[
\begin{align*}
A_{11} (u_{ss} - R^{-1} w_s) + D_{11} R^{-2} (u_{ss} + R w_{sss}) &= I_0 \ddot{u}, \\
- A_{11} (R^{-1} u_s - R^{-2} w) + D_{11} (w_{sss} + R^{-1} u_{sss}) &= -I_0 \ddot{w}.
\end{align*}
\]

The \( A_{11} \) and \( D_{11} \) are the axial and flexural stiffness of the shell, defined as \( A_{11} = E h / (1 - v^2) \) and \( D_{11} = E h^3 / 12(1 - v^2), \) where \( h \) is the thickness of the shell. The \( I_0 \) is the first moment of mass defined as \( \rho h. \) The associated essential and natural boundary conditions are

\[
\begin{align*}
u \text{ is prescribed or } Q_u &= A_{11} (u_s - R^{-1} w) + D_{11} R^{-1} (w_{ss} + R^{-1} u_s), \\
w \text{ is prescribed or } Q_w &= -D_{11} (R^{-1} u_s + w_{ss}), \\
w_s = \psi \text{ is prescribed or } Q_\psi &= D_{11} (R^{-1} u_s + w_{ss}),
\end{align*}
\]

where \( Q_u, Q_w \) and \( Q_\psi \) are the external forces corresponding to the \( u, w \) and \( \psi \) degree of freedom, respectively.

The multiple-elastic shell model for \( N \)-walled CNT (based on Eqs. (6) and (7)) is governed by the following set of \( 2N \)-coupled equations:

\[
\begin{align*}
A_{11}^1 (u_{1,ss} - R_1^{-1} w_{1,s}) + D_{11}^1 R_1^{-2} (u_{1,ss} + R_1 w_{1,sss}) - I_0^1 \ddot{u}_1 &= 0, \\
- A_{11}^1 (R_1^{-1} u_{1,s} - R_1^{-2} w_1) + D_{11}^1 (w_{1,sss} + R_1^{-1} u_{1,sss}) + I_0^1 \ddot{w}_1 &= c_1 (w_2 - w_1),
\end{align*}
\]
where \( w_p(s,t) \) and \( u_p(s,t) \) are the deflections of the \( p \)th CNT and the superscripts denote the material and geometric properties of the \( p \)th tube. For CNT, the Young's modulus \( E = 1 \) TPa (with the effective thickness 0.35 nm) and the mass density \( \rho = 1.3 \) g/cm\(^3\). The interaction coefficients \( c_p(p = 1, \ldots, N - 1) \) can be estimated approximately as (Ru, 2000a)

\[
c_p = \frac{400R_p \text{erg/cm}^2}{0.16d^2}, \quad d = 0.142 \text{ nm}, \quad p = 1, \ldots, N - 1.
\]

The coefficients \( c_p \) have been estimated as the second derivative of the energy-interlayer spacing relations of two flat monolayers i.e., it does not take the curvature effect of CNTs into account.

### 2.1. Computation of the wave numbers and speeds

The spectral formulation begins by assuming the displacement as a synthesis of plane waves of the form

\[
u_n = \sum_{n=1}^{N_q} \tilde{u}e^{-j(kx + \omega_n t)}, \quad w_n = \sum_{n=1}^{N_q} \tilde{w}e^{-j(kx + \omega_n t)},
\]

where \( k \) is the wave number, \( \omega_n \) is the circular frequency of the \( n \)th sampling point and \( j^2 = -1 \). The \( N_q \) is the frequency index corresponding to the Nyquist frequency in Fast Fourier Transform (FFT) and inverse-FFT used for conversion between time and frequency domain. When Eq. (18) is substituted in Eqs. (11)–(16) the resulting discretized form can be written as a polynomial eigenvalue problem (PEP)

\[
(k^4 A_4 + k^3 A_3 + k^2 A_2 + k A_1 + A_0)\nu = W\nu = 0, \quad A_p \in \mathbb{C}^{2N \times 2N}
\]

and \( \nu \) are the unknowns \( \{u_1, w_1, \ldots, u_N, w_N\} \). The matrices \( A_p \) are best described by the following rules (while \( p \) ranges from 1 to \( N \)):

\[
A_1(2p, 2p) = D_{11}^p R_p^2, \quad A_3(2p - 1, 2p) = jD_{11}^p R_p = A_3(2p, 2p-1),
\]

\[
A_2(2p - 1, 2p - 1) = -D_{11}^p R_p^2 - D_{11}^p, \quad A_4(2p - 1, 2p) = jA_{11}^p R_p = A_4(2p, 2p - 1).
\]

Further, the matrix \( A_0 \) can be decomposed as \( A_0 = B_0 + B_1 + \omega^2 M \), where \( B_0(2p, 2p) = A_{11}^p, \quad p = 1, \ldots, N \) and

\[
B_1(2p, 2p) = c_y R_p^2, \quad B_1(2p, 2p + 2) = -c_y R_p^2,
\]

\[
B_1(2p + 2, 2p + 2) = -c_y R_p^2, \quad B_1(2p + 2, 2p + 2) = B_1(2p + 2, 2p + 2) + c_y R_p^2.
\]

where \( p \) ranges from 1 to \( N - 1 \). Thus, the matrix \( B_1 \) contains the coupling terms of the governing equations.

Solving the PEP as described in Eq. (19), the eigenvalues \( k \) and the eigenvectors \( \nu \) are obtained, which will be used in subsequent element formulation. As the \( A_4 \) matrix is singular, the lambda matrix \( W \) is not regular and admits infinite eigenvalues (Lancaster, 1969). As the order of the matrices and the PEP suggest, the PEP yields \( 2N \times 4 \), i.e., \( 8N \) wave numbers. However, only \( 6N \) of them are finite as can be found in the numerical computation, which cover the complete solution space. Thus, for a \( N \)-walled nanotube there are \( 6N \) wave numbers and \( 2N \) phase speeds \( (c_{p}) \) and group speeds \( (c_{g}) \). The phase speeds are defined as \( \omega/k \) and the group speeds are defined as \( d\omega/dRe(k) \), \( Re \) denotes the real part of a complex number. In case of beam approximation, the group speeds were computed from the dispersion relation. Here, because of its complexity, they will be computed by directly appealing to their definitions.

### 2.2. Computation of the cut-off frequencies

Compared to the beam model, where \( N \)-walled CNT has \( N - 1 \) cut-off frequencies (where the wave number is zero and thus, group speed is zero and phase speed is infinite), in this model, an \( N \)-walled CNT has, in
general, \( N \) cut-off frequencies. These frequencies are obtained from the dispersion relation by substituting \( k = 0 \). As shown in the beam model, the cut-off frequency computation is another PEP

\[
(B_0 + B_1 + \omega^2 M)x = 0,
\]

where \( x \) is a hypothetical eigenvectors of no consequence in our subsequent formulation. For \( N = 1 \), the expression of cut-off frequency is given in Doyle (1997), which is same as that for a curved beam. For \( N = 2 \), although the expression is in analytic form it is avoided here because of its complexity.

### 2.3. Computation of the wave amplitudes

The wave amplitudes are computed by posing the PEP as a Generalized Eigenvalue Problem (GEP). The generalized (linearized) version of the problem equation (19) takes the form

\[
Cz = \lambda Dz,
\]

where

\[
C = \begin{bmatrix}
0 & I & 0 & 0 \\
0 & 0 & I & 0 \\
0 & 0 & 0 & I \\
-A_0 & -A_1 & -A_2 & -A_3
\end{bmatrix},
D = \begin{bmatrix}
I & 0 & 0 & 0 \\
0 & I & 0 & 0 \\
0 & 0 & I & 0 \\
0 & 0 & 0 & A_4
\end{bmatrix}.
\]

Here \( I \) and \( 0 \) are, respectively, the identity and zero matrix of size \( 2N \times 2N \). The GEP can be solved by several existing algorithms, however, in this case the QZ factorization based method is used. The eigenvectors of the original problem (\( v \) in Eq. (19)) is recovered from the eigenvectors of the linearized problem (\( z \) in Eq. (25)) by the relation

\[
z = (v^T, k_1v^T, k_2v^T, k_3v^T)^T,
\]

where (\( )^T \) denotes the transpose of a matrix. Only those columns of \( z \) are chosen that correspond to finite eigenvalues. This yields the required set of finite eigenvectors of the original problem, \( U \), which is of dimension \( 2N \times 6N \).

Another method of finding the eigenvalues and eigenvectors is the method of SVD. Here, the original PEP is identified as the problem of finding the null space of \( W \) Eq. (19). As we are interested in the non-trivial solution for \( v \), the lambda matrix \( W \) should be singular. This singularity is achieved by solving the equation \( \det(W) = 0 \), which generates the characteristic equation for the eigenvalues \( k \). Let us denote the finite roots as \( k_i \), \( i = 1, \ldots, 6N \). For these values of \( k \), the matrix \( W \) is singular, i.e., the null space of \( W \) is non-trivial and \( v \) lies in this space. To find out the elements of the null-space, we take the help of the SVD. According to the SVD theorem, any rectangular complex valued matrix can be decomposed in terms of two unitary matrices \( U \) and \( V \) and a diagonal matrix \( S \) as

\[
W = USV^H,
\]

where (\( )^H \) denotes the Hermitian conjugate of a matrix. The \( S \) is the matrix of singular values, where at least one diagonal element will be zero as \( W \) is singular. The most important property of this decomposition relevant here is that the columns of \( V \) that correspond to the zero singular values (zero diagonal elements of \( S \)) are the elements of the null-space of \( W \). Thus for each \( k_i \), the null space members \( v \in \mathbb{C}^{2N \times 1} \) are computed (selected from \( V \)) and stored in the array \( \Phi \in \mathbb{C}^{2N \times 6N} \). Further details on this aspect can be found in the beam model work (Chakraborty et al., 2006).

Once the wave amplitudes \( \Phi \) are obtained the solution can be written as

\[
\{\tilde{u}_1, \tilde{w}_1, \ldots, \tilde{u}_N, \tilde{w}_N\} = \Phi L a, \quad \Phi \in \mathbb{C}^{2N \times 6N}, \quad L \in \mathbb{C}^{6N \times 6N}, \quad a \in \mathbb{C}^{6N \times 1},
\]

where \( L(p, p) = \exp(-jk ps), \quad p = 1, \ldots, 6N \) and the \( a \) are the unknown coefficients to be determined. Two different elements can be prepared using this solution.
2.4. Finite length spectral element

For this element, the complete solution in Eq. (29) is considered, i.e., both the forward and backward moving waves are considered. The unknowns, am-s are to be replaced by the nodal variables, which are the displacements in the X–Z-plane (u and w) and the rotation for each wall ψ = ψs. Thus, each node has 3N degrees of freedom (dofs) and the two nodal element has 6N dofs. The nodal variables in the first and second node are arranged as \{u1, w1, ψ1, . . . , uN, wN, ψN\} and they are collectively referred as u1 and u2, for node 1 (s = 0) and node 2 (s = L), respectively. Using Eq. (29), the relation between u1, u2 and a are expressed as

\[ \bar{u} = \{u_1; u_2\} = T_1a, \quad T_1 \in \mathbb{C}^{6N \times 6N}, \]

where the elements of the T1 matrix can be given by the rule

\[ T_1(3p - 2, q) = \Phi(2p - 1, q), \quad T_1(3p - 1, q) = \Phi(2p, q), \]
\[ T_1(3p, q) = -j\Phi(2p, q)k_p, \quad \text{where } p = 1, \ldots, N, \quad q = 1, \ldots, 6N, \]
\[ T_1(p + 3N, q) = T_1(p, q) \exp(-jk_qL), \quad \text{where } p = 1, \ldots, 3N, \quad q = 1, \ldots, 6N. \]

Next, the relation between the nodal forces and the coefficients needs to be established. The nodal forces are axial (hoop) force \(Q_a\), shear force \(Q_w\) and bending moment \(Q_\psi\), which are defined earlier. At each node there are 3N such forces which are given as (where p ranges from 1 to N)

\[ Q^p_a = A^p_{11}(up_s - R^{-1}_p w_p) + D^p_{11}R^{-1}_p(w_{p,ss} + R^{-1}_p u_{p,s}), \]
\[ Q^p_w = -D^p_{11}(R^{-1}_p u_{p,s} + w_{p,ss}), \quad Q^p_\psi = D^p_{11}(R^{-1}_p u_{p,s} + w_{p,ss}). \]

Using the above relationship, the nodal forces \(f_1\) and \(f_2\) are evaluated at node 1 (s = 0) and node 2 (s = L), respectively, as

\[ f_1 = \{-Q^0_a(0), -Q^0_w(0), -Q^0_\psi(0), \ldots, -Q^0_a(L), -Q^0_w(L), -Q^0_\psi(L)\}, \]
\[ f_2 = \{Q^1_a(L), Q^1_w(L), Q^1_\psi(L), \ldots, Q^1_a(L), Q^1_w(L), Q^1_\psi(L)\}, \]

which are related to the coefficients a by the relation

\[ \bar{f} = \{f_1; f_2\} = T_2a, \quad T_2 \in \mathbb{C}^{6N \times 6N}. \]

Fig. 2. Wave number variation for N = 2 (shell theory).
The elements of $T_2$ are given by the rule

$$T_2(3p - 2, q) = -A_{11}^q (-j\Phi(2p - 1, q)k_q - R_p^{-1}\Phi(2p, q)) - D_{11}^p R_p^{-1}(-\Phi(2p, q)k_q - jR_p^{-1}\Phi(2p - 1, q)k_q),$$

$$T_2(3p - 1, q) = -R_p^{-1}D_{11}^p \Phi(2p - 1, q)k_q^2 + jD_{11}^p \Phi(2p, q)k_q^3,$$

$$T_2(3p, q) = jR_p^{-1}D_{11}^p \Phi(2p - 1, q)k_q + D_{11}^p \Phi(2p, q)k_q^2.$$  \hspace{1cm} (39)

Combining Eqs. (30) and (38), the relation between the nodal forces and the nodal displacements is

$$\tilde{f} = T_2T_1^{-1}\tilde{u} = K\tilde{u},$$  \hspace{1cm} (40)

Combining Eqs. (30) and (38), the relation between the nodal forces and the nodal displacements is

$$\tilde{f} = T_2T_1^{-1}\tilde{u} = K\tilde{u},$$  \hspace{1cm} (41)

Fig. 3. Wave number variation for $N = 2$ (beam theory).

Fig. 4. Phase speed variation for $N = 2$ (shell theory).
where $K$ is the dynamic stiffness matrix of size $6N \times 6N$. This matrix exactly relates the nodal forces with nodal displacements at frequency $\omega_n$. Thus, one element is sufficient to model a MWNT of any number of walls.

2.5. Semi-infinite spectral element

While forming the total solution, if only the forward propagating components are considered, the waveguide will resemble to an infinite length circular structure, i.e., a helix, which carries no reflection from the

![Fig. 5. Phase speed variation for $N = 2$ (beam theory).](image1)

![Fig. 6. Group speed variation for $N = 2$ (shell theory).](image2)
other boundary. This element is also called throw-off element as it acts as a conduit for throwing away energy from the structure. The element is useful in modelling large structures and to introduce artificial damping. The displacement field for this element is

\[ \{\hat{u}_1, \hat{w}_1, \ldots, \hat{u}_N, \hat{w}_N\} = \Phi L a, \quad \Phi \in \mathbb{C}^{2N \times 3N}, \quad L \in \mathbb{C}^{3N \times 3N}, \quad a \in \mathbb{C}^{3N \times 1}, \]

which can be used to establish the relation between the nodal displacements and forces as

\[ \tilde{u} = u_1 = T_1 a, \quad \tilde{f} = f_1 = T_2 a, \quad f = T_2 T_1^{-1} u = Ku, \]

where all the matrices are now of size \( 3N \times 3N \).

3. Numerical analysis

In this section, the efficiency of the developed spectral element is demonstrated. First, the wave number, phase speed and group speed variation is investigated for different wall numbers. Then the effect of wall-number on the cut-off frequencies is studied. Finally, a broad-band pulse loading is applied to study the wave propagation in MWNT.

For all the subsequent numerical examples, MWNT is considered with \( E = 1 \) TPa, \( \nu = 0.3 \) and \( \rho = 1300 \) kg/m\(^3\). The innermost radius of the tube is taken as 5 nm and each tube is 0.35 nm thick. The van der Waals force interaction coefficient for the first wall becomes 0.62 TPa. The geometric and material properties result waveforms and wave characteristics, which are given in the following sections.

3.1. Spectrum and dispersion relation

The wave numbers, phase speed and group speed variation for \( N = 2 \) are plotted in Figs. 2–6, respectively. As previously mentioned, there are two cut-off frequencies, one at 0.8140 and another at 1.6438 THz. The blue\(^1\) lines denote the real part of the wave numbers and the black lines denote the imaginary parts. At any frequency, there are purely real wave numbers (propagating), purely imaginary (evanescent) wave numbers and complex modes (inhomogeneous waves), which attenuate while propagating. It is very difficult to identify how many pure real or imaginary modes there. At most, it can be said from Fig. 2 that initially there are ten propagating/inhomogeneous modes and four inhomogeneous modes. However, afterwards, there are six inhomogeneous modes and six propagating modes. After the second cut-off frequency, two more propagating modes come up and thus, there are four inhomogeneous modes and eight propagating modes.

In comparison, the spectrum relation predicted by the Euler–Bernoulli theory is much simpler Chakraborty et al. (2006). There are eight modes although only two base wave numbers are shown in Fig. 3. The other wave numbers can be found from these by multiplying them by \(-1\) and \(\pm j\). Thus, two of them are always propagating (and two are always evanescent) and two propagate (and attenuate) once the frequency exceeds the cut-off frequency of 1.432 THz.

The phase and group speed variations (dispersion relation) deal only with the real part of the wave numbers. Thus, the phase speed variation (Fig. 4) initially shows five modes, which in the later stage becomes four. These four speeds are coming from the eight propagating modes (half of them are forward moving and half backward). The same idea is reflected in the group speed variation also (Fig. 6), where the four propagating modes are easily discernible. Further, it can be seen that at the cut-off frequencies, the phase speeds are escaping to infinity, whereas, the group speeds are becoming zero. Two sets of speeds can be identified in the dispersion relations, one that has an average value of 24 km/s and the other set contains two values 49 and 54 km/s. If the phase speed predicted by the beam theory is compared (given in Fig. 5) it can be inferred that the beam theory fails to predict the slower propagating modes, although the higher modes are captured quite accurately.

For \( N = 5 \), the spectrum and dispersion relations are very complicated as can be seen in Figs. 7–11. There are four cut-off frequencies at 0.7514, 1.2587, 1.6162 and 1.8359 THz. Thus, it is not necessary to have as many

\(^{1}\) For interpretation of color in Figs. 2–15, the reader is referred to the web version of this article.
cut-off bending modes as the number of walls. In fact, for \( N = 10 \), there are eight cut-off frequencies. The cut-off frequencies predicted by the beam theory are at 0.6297, 1.194, 1.643 and 1.932 THz, which are very close to that predicted by the shell theory (see Fig. 8). It is to be noted that the beam wave number magnitudes are bounded by 0.4 nm\(^{-1}\), i.e., there is no mode close to the higher valued shell wave numbers (greater than 0.5 nm\(^{-1}\)). This explains the absence of low phase speed in the dispersion relation of beam given in Fig. 10. The values predicted are however, lower than the five shell phase speeds given in Fig. 9. The rest five phase speeds have an average value of 26.1382 km/s and hence it is clear that they correspond to the \( u \) dof. Thus, the present shell model captures the first symmetric Lamb wave mode of MWNT, which beyond the realm
of the beam theory. The group speeds are given in Fig. 11, which clearly shows the presence of first symmetric ($s_0$) and anti-symmetric mode ($a_0$). It is also evident from the figure that the $a_0$ modes are increasing with frequency, i.e., dispersive, whereas, the $s_0$ modes are constant at high frequency.

As happened in the beam model, the current spectrum relation also suggests an upper and lower bound for the cut-off frequencies as the wall number increases. The variations of the maximum and minimum cut-off frequencies are shown in Fig. 12. The estimation by beam theory is also included in the same figure (shown in firm line). As the figure suggests, the maximum cut-off frequency predicted by the shell theory is
1.864 THz, whereas, the beam theory predicts a value of 2.085 THz. Thus, the beam theory overestimates the cut-off frequency almost by 12%. The minimum cut-off frequency variation does not follow the same continuous variation as in the beam theory case. However, in absence of uniform convergence, the minimum value seems to be around 0.2 THz whereas, for beam theory it is only 0.03 THz.

3.2. Effect of broad-band pulse loading

The developed element is suitable for modelling and analysis of MWNT for broad-band loading with relatively marginal cost of computation as compared to any other method. This capability is demonstrated in this
example. A MWNT is considered, which is loaded in the transverse direction throughout its length. The tube is modelled by 2 elements and it takes on average 30 s to perform the simulation. The load is having a frequency content of around 5 THz (see Fig. 13), whose time domain representation is shown in the inset. The transverse displacement and velocity measured at the innermost wall are presented in Figs. 14 and 15 for single wall and double wall nanotube. As the figure suggests, with increasing wall number the stiffness of the nanotube increases. This is evident in the lower value of the displacement and velocity for $N = 2$ as compared to the $N = 1$ case.

Fig. 13. Broad-band pulse loading.

Fig. 14. Transverse displacement variation for different wall number.
4. Conclusion

A new spectral element is formulated based on the plane-strain shell theory, which can efficiently model MWNTs. The element can have any number of walls and the essential wave propagation characteristics, in terms of spectrum relation, dispersion relation and cut-off frequencies are inbuilt in the element formulation. The formulation reveals the complicated nature of the wave number, phase and group speed variation over the number of walls, $N$. It is found that for small values of $N$, the number of cut-off frequencies is equal to $N$, as opposed to the previous beam model. However, for higher values of $N$, there can be $N - 1$ or $N - 2$ cut-off frequencies. Like the beam model, the cut-off frequencies are bounded above, although, no exact lower bound could be obtained. It is shown that, the beam theory overestimates the cut-off frequency. Further, the shell model captures the first symmetric Lamb wave mode, which is not present in the earlier beam model of MWNT. The study of broad-band loading shows the effect of increasing $N$ in terms of increasing stiffness of the structure.

References


