Modelling carbon nano-tubes dynamical behaviour via nonlocal theory – free vibrations and dispersion relations

A. Muc
Institute of Machine Design, Cracow University of Technology, Kraków, Poland
olekmuc@mech.pk.edu.pl

Abstract. In the present paper the influence of non-local gradient formulations on the dynamical behaviour (free vibrations and dispersion relations) of carbon nanotubes analysed with the use of 2D shell theory is discussed. At the beginning the compact, consistent approach to the nonlocal (the Mindlin-Tiersten theory) description of 2D carbon nanoshells is shown. The presented results demonstrate the equivalence of free vibration analysis to the normal displacement mode (RBM) of carbon nanoshells. The possible extension of the presented formulations are also discussed.

1. Introduction

New materials and constructions involve a lot of problems that cannot be solved in the frame of classical continuum mechanics not saying about various new computational problems arising in the analysis. Atomic and electron structure in nano-size materials, such as nano-shells, nano-plates, nano-ribbons, nano-/micro-porous functionally graded materials or 1D, 2D, 3D quantum dots (QDs) are strongly affected by the necessity of the use of different formalisms including also quantum mechanics or quantum field theory methods – see e.g. Muc, Banaś [1].

For mechanical modeling of the nano-beams, plates or shells, the classical (understood and called as local) continuum 2D or 3D models are deemed to fail, because these models are described/characterized by global material properties only and properties that are related to micro- / nano-structures are neglected. Hence, these local theories are unable to depict (with the required accuracy) the influence of nano-scale effects when the size of a body enters into the micro- or nano-dimension. While the sizes of the system we study (so-called characteristic lengths) are comparable in size to the investigated structures the theoretical and numerical approaches have an accuracy similar to first principle quantum mechanical methods. Considering nano or QD structures it becomes necessary to analyse the influences of the length scale parameter/parameters on static and dynamic behaviour of constructions. The present state-of-the-art demonstrates evidently that there are various approaches that try to solve the above-mentioned problems:

- to incorporate and adopt the non-local formulations existing in the classical mechanics – the comparison of those methods is discussed by Raffi-Tabar et al. [2] and Muc [3]
- to apply dynamic simulation methods in order to model nano-size structures and then to solve problems with the use of computer methods – the presentation of those methods is given in Refs [4-6],
to implement more parameters into existing plate or shell theories – the examples of such modifications are presented e.g. by Shahverdi, Barati [7] or the theory of micromorphic continuum Leismann, Mahnken [8].

Researchers applied various types of elasticity theories for the vibration analysis of the nanostructures in more recent years. Liew and Wang [9] presented a broad review of literature dealing with the wave propagation in carbon nanotubes. However their attention is mainly focused on the research of thick shells. They pointed out that it is necessary to analyse carbon nanostructures in the terahertz frequency range. The similar conclusions were drawn in the numerical computations carried out by Muc [4-6] using anisotropic shell models based on the first order transverse shear shell deformation theory. The similar model was also implemented by Ghavanloo, Fazelzadeh [10]. Investigations of vibrational characteristics of nanostructures were also conducted with the use of non-local theories applied in single- or double-walled carbon nanotubes - Hu et al [11], Natsuki et al. [12] and Ghorbanpourarani et al. [13]. The analysis was also extended to the description of dynamical behaviour of doubly-curved nano-shells – Dindarloo and Li [14]. It should be pointed out that the majority of papers employed the Eringen formulation (operator) only as e.g. Sayyid, Hashemi Kachapi [15, 16] in the analysis of carbon nanotubes with piezoelectrics and resting on the Pasternak foundation.

The fundamental aim of the present paper is following: to present in a compact and concise manner the comparison of the results for various formulations of non-local theories (both the Eringen and the Mindlin-Tiersten approach) in view of carbon nanotubes free vibrations behaviour and vibration dynamics understood in the sense of dispersion curve distributions. The advantage of the proposed formulation and approach lies in the direct implementation of two length parameters, separately for the gradient stress and strain non-local continuum theories.

2. Governing equations

A broad discussion of modeling carbon nanotubes (CNTs) using classical shell formulations is conducted in Ref [17]. The implementation of non-local, gradient formulations of various shell structures behaviour is formulated by Muc [3, 18].

The general scheme of building 2D approximations of beam/plates/shell structures theories is shown in figure 1. The inclusion of gradient theories (the Mindlin’s-Tiersten theory [19]) is carried out by the Laplacian operators written in the following way:

\[ L^{(E)} = (1 - f^{(E)} \Delta) \]

![Figure 1. Continuum model of carbon nanotube’s structure](image)
They are called as the linear Aifantis (Eringen) differential operators, and $\Delta$ means the Laplacian operator, whereas $l^{(E)}$ is the length scale parameter.

3. **Natural frequencies of carbon nanotubes**

In the description of CNTs cylindrical shells deformations the simplest form of the kinematical hypothesis is employed. The shells are characterized by three parameters: $u_1$ – the longitudinal ($x_1$) displacements, $u_2$ – the circumferential ($x_2$) displacements and $u_3$ – the normal (radial $x_3$) displacements. The properties of the graphene constituting the nanoshells are following: the thickness $t = 0.34$ nm, the length $L = 10$ nm, the Young modulus $E = 1.06$TPa and the Poisson ratio $\nu = 0.25$.

In the non-local formulation the governing relations characterizing free vibrations of cylindrical shells are written in the following way:

$$L^4 L_{ij} u_i = \delta_{ij} \rho h L^E \frac{\partial^2 u_i}{\partial x_i^2}, L_{ij} = L_{ji}, i, j = 1, 2, 3$$

(2)

where $\delta_{ij}$ is the Kronecker symbol and $L_{ij}$ are differential operators listed as below:

$$L_{11} / h = C_{11} \frac{\partial^2}{\partial x_1^2} + C_{66} \frac{\partial^2}{\partial x_2^2}, L_{12} / h = (C_{12} + C_{66}) \frac{\partial^2}{\partial x_1 \partial x_2}, L_{13} = \frac{h}{R} C_{12} \frac{\partial}{\partial x_1},$$

$$L_{22} / h = \left(1 + \frac{12h^2}{R^2}\right) \left(C_{66} \frac{\partial^2}{\partial x_1^2} + C_{11} \frac{\partial^2}{\partial x_2^2}\right),$$

$$L_{23} = \frac{hC_{11}}{R} \frac{\partial}{\partial x_2} - \frac{h^3}{12R} \left[C_{12} + 2C_{66}\right] \frac{\partial^3}{\partial x_1^2 \partial x_2} - C_{11} \frac{\partial}{\partial x_2},$$

$$L_{33} = \frac{hC_{11}}{R^2} \frac{\partial^3}{\partial x_1 \partial x_2^2} - \frac{2}{12R} \left[C_{12} + 2C_{66}\right] \frac{\partial^4}{\partial x_1^2 \partial x_2^2},$$

(3)

$$C_{11} = C_{22} = E/(1-\nu^2), C_{12} = \nu C_{11}, C_{44} = C_{55} = C_{66} = 0.5(1-\nu)C_{11}$$

Let us assume that all displacement functions are represented by the relations: $u_i(x_1,x_2,t)=U_i(x_1,x_2)\sin\omega t$. It is well-known that the normal vibrational modes are dominant for the lower eigenfrequencies $\omega$. Therefore, it is convenient to reduce the governing system of equations to one having one function only $U_3$ (normal nano-shell deflection). As usual the solution depends on the form of boundary conditions. Assuming the simply supported boundary conditions, i.e.

$$U_3(x_1,x_2)=\sum_{\alpha_1=0}^{m-1} W_{\alpha} \sin(\alpha_m x_1)\sin(\beta_n x_2), \quad \alpha_m = m \pi / L, \quad \beta_n = n \pi / R, \quad m, n = \text{natural wavenumbers}$$

the solution (the normal eigenfrequencies) can be written in the following way:

$$\omega^2(\text{NonlocalTheory}) = \left[1 + l^{(E)} \left(\alpha_m^2 + \beta_n^2\right)\right] \left[\frac{C_{11}}{12} \frac{h^2}{R^4} \left(\alpha_m^2 + \beta_n^2\right)^2 + \frac{R^2 \alpha_m^4}{\left(\alpha_m^2 + \beta_n^2\right)^2}\right]$$

(4)

The presented by Eq.(4) effects of the application of the non-local theories are illustrated in figure 2. Using the gradient strain theory one can observe the increase of natural frequencies (and similarly buckling loads) in the comparison with the results for the gradient stress theory. The influence of both non-local formulations is the function of two parameters $l^{(E)}$ and $l^{(D)}$. The identical conclusions to the above were drawn for carbon nano-ribbons Ref [3] and for carbon nano-beams [20]. However, it should be emphasized that the values of multipliers $1 + l^{(E)} (\alpha_m^2 + \beta_n^2)$ and $1 + l^{(D)} (\alpha_m^2 + \beta_n^2)$ are different for nano-ribbons and nano-shells since the values of wavenumbers $m$ and $n$ are not identical for shallow and deep cylinders – the broader explanations of those effects is presented in Ref [21] (see figure 2).
4. Dispersion relations for single walled carbon nanotubes

In dynamic problems for cylindrical shells, similarly as for isotropic structures (see e.g. Refs [22-25]), the influence of non-local/gradient formulations can be assessed and evaluated by the investigated dispersive properties of CNTs. Although the implemented methods of the analysis are identical to those proposed e.g. by Karczub [26] (the package Mathematica) the inclusion of the gradient theories significantly enriches the previous considerations.

As it is demonstrated e.g. in Ref [25] in order to build an appropriate dispersion relations it is necessary to transform the relations from time and displacement space into more convenient frequency and wavenumber space (Skelton, James [27]). Usually, it can be achieved by the following classical transformation:

\[ f(x, \phi, t) = \sum_{n=-\infty}^{\infty} e^{i\phi} \int_{-\infty}^{\infty} \int F(\alpha, n, \omega) e^{i(\alpha x_n - \omega t)} d\alpha d\omega, \phi = x_2 l R \]  \hspace{0.5cm} (5)

Inserting the above in Eqs (2), (3) one can find the relation:

\[
\begin{bmatrix}
\hat{L}_1(s,n) \\
\hat{L}_2(s,n) \\
\hat{L}_3(s,n)
\end{bmatrix}
\begin{bmatrix}
U_1(s,n,\Omega) \\
U_2(s,n,\Omega) \\
U_3(s,n,\Omega)
\end{bmatrix}
= \Omega^2 \delta_{kl} \left[ 1 + l^2 \left( s^2 + n^2 \right) \right] \begin{bmatrix}
U_1(s,n,\Omega) \\
U_2(s,n,\Omega) \\
U_3(s,n,\Omega)
\end{bmatrix} e^{i(\alpha x_n - \omega t)} e^{in\phi} = 0, \hspace{0.5cm} (6)
\]

\[
\hat{L}_k(s,n) = L^A L_k e^{i(\alpha x_n - \omega t)} e^{in\phi}, \hspace{0.5cm} k,l = 1,2,3, \Omega = R\omega l c_L, c_L = \sqrt{C_{11}/\rho}, s = R\alpha \hspace{0.5cm} (7)
\]

The nonzero solutions \(U_k\) exist as \(\text{Det} [\text{matrix in the bracket } \{\ldots\}]\) in Eq. (6). Notice that the relation (5) corresponds to the assumed form of the free vibration analysis described in the previous section. The condition \(\text{Det}[\ldots]=0\) allows us to determine the relationship between \(s\) and \(\Omega\) so called as dispersion relations of cylindrical nanoshells in the nonlocal Mindlin’s formulation. For the prescribed value of the frequency \(\Omega\) the solutions with respect to the values \(s\) and \(n\) can be evaluated using the symbolic package Mathematica.

For cylindrical nanoshells let us note that in the literature the dispersion relations were evaluated for torsional modes – Hu et al. [10] using the Enringen nonlocal formulations and for radial modes.

For \(n=0\) one can distinguish: 1) breathing-modes (longitudinal and radial displacements), 2) a torsional-mode (circumferential displacements). For \(n>0\) different branches of the dispersion curves are usually estimated.
The influence of employing the non-local formulations is shown in figure 3. Similarly as for free vibrations the use of the Eringen stress gradient theory decreases values of frequencies \( \omega \) (in the comparison to the classical theories), whereas the Aifantis strain gradient theory have opposite effects. The magnitude of the growth/decrease is a function of the length scale parameters \( t^E, l^E \) defined in Eq. (1). The use of the Mindlin theory does not change values of frequencies since \( l^A = l^E \). In general, the Mindlin model, unifies the gradient elasticity theories of Eringen and Aifantis. Let us note that different branches (modes) of the solution of Eq. (6) can be plotted in plots \( \omega \)-s for different values of \( n \).

As it may be observed in figures 2 and 3 the non-local gradient theories results in the increase of the dynamical effects (eigenfrequencies or spectral distributions) for the Aifantis formulation or decrease for the Eringen theory. The increase/decrease factor is strongly dependent on the assumed values of the length scale – see Eq. (1). The presented results are also strongly affected by form of the applied shell theory. The present results are based on the use of the Love-Kirchhoff hypothesis due to the prescribed values of the thickness ratio \( t/L = 0.034 \). The fundamental relations (3), (6) will be changed significantly for transverse shear shell deformation theories.

5. References

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