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Ritz formulation for the wave propagation analysis of axially functionally graded carbon nanotubes

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ABSTRACT

Longitudinal wave propagation in axially functionally graded carbon nanotubes was investigated using three different solution methods: analytical, higher order Haar wavelet and Ritz methods. The results of the various solution methods were compared and validated. A weak form solution for the wave frequency was presented using the Lagrangian energy functional and the Ritz method. Exponential and power-law material grading variations were considered. Material grading parameters and grading nonlocality effects on the axial wave propagation frequency were investigated. The present study could be useful in the wave dynamic analysis of axially graded nanostructures.

1. Introduction

Functionally graded nanostructures have become popular in recent years. Designable material properties are the most important advantage of the functionally graded materials. Axially graded carbon nanotubes (CNTs) are a type of these materials and have great potential in the production of fiber optics with improved signal transmission capabilities [1].

Wave propagation in nanoscale structures has been an interesting topic discussed by scientists for the last 70 years. Eringen mentioned this important issue in his well-known "nonlocal elasticity theory" [2], which he developed in the 1960s. Wave propagation in axially graded nanostructures has different characteristics and should be investigated using the continuum mechanics approach. Wave propagation in axially graded rods has been investigated in the previous work of Xue and Pan [3]. At the nanoscale, Narendar [4] studied the elastic wave propagation in exponentially graded magneto-electro-elastic nanorods. The micropolar finite element method for wave propagation analysis in variable cross-sectional nanorods was proposed in [5]. Functionally graded nanostructures [6] and CNT-reinforced composites [7] have been studied by researchers.

The present study investigates the wave propagation solution of axially graded CNTs. Material properties such as Young's modulus, density and nonlocality are examined in an axially functionally graded form. Grading nonlocality has been rarely studied in the literature. Weak energy formulation and the nonlocal elasticity theory are used together in the modeling of wave dynamics. The approximate Ritz method is used in the solution of the wave equation.

2. Analysis

In the present study, the CNT with axially graded material properties is modeled as an axially functionally graded hollow rod. According to the Cartesian coordinate system, *x*-axis is in the length direction. Longitudinal (u(x,t)) displacement of the rod is defined using the Rayleigh rod theory [8]:

$$u = u(x, t), \tag{1}$$

where t is time. Axial strain (ε_{xx}) and stress (σ_{xx}) relations of the rod are defined as:

$$\varepsilon_{xx} = \frac{\partial u(x,t)}{\partial x} , \quad \sigma_{xx} = E(x)\varepsilon_{xx},$$
 (2)

where E(x) is the Young's modulus of the rod. Because of the length scale effect at the nanoscale, size-dependent nonlocal theories should be used in the continuum modeling of nanostructures.

2.1. The nonlocal elasticity theory

To capture the size effect at the nanoscale, Eringen's nonlocal constitutive relation for stress gradient elasticity can be defined as [2]:

$$(1 - \mu(x)\nabla^2)\tau_{kl} = \lambda\varepsilon_{rr}\delta_{kl} + 2G\varepsilon_{kl},\tag{3}$$

where τ_{kl} is the nonlocal stress tensor, ε_{rr} is the sum of normal strains, δ_{kl} is the Kronecker delta, ε_{kl} is the strain tensor, λ and *G* are the Lamé constants, and $\mu(x)$ is called the nonlocal parameter. Equation (3) can be written in the following one-dimensional form using Eq. (2) for the axially graded CNT:

$$\left(1-\mu(x)\frac{\partial^2}{\partial x^2}\right)\sigma_{xx} = E(x)\varepsilon_{xx}.$$
(4)

2.2. Nonlocal energy formulation of the Rayleigh nanorod

In the framework of the nonlocal Rayleigh rod theory, potential and kinetic energies of the nanorod can be written as [9]:

$$U = \int_0^a E(x) A\left(\frac{\partial u(x,t)}{\partial x}\right)^2 dx, \qquad (5)$$

$$T = \int_0^a \rho(x) A\left(\frac{\partial u(x,t)}{\partial t}\right)^2 dx - \int_0^a \mu(x) \frac{\partial}{\partial x} \left(\rho(x) A \frac{\partial u(x,t)}{\partial t}\right) \frac{\partial^2 u(x,t)}{\partial x \partial t} dx,$$
(6)

where U and T are defined as the potential and kinetic energies of the nanorod, and a is the internal characteristic length, which is the distance between two atoms. The Lagrangian energy functional of the CNT can be defined using potential and kinetic energies:

$$L = T - U = \int_0^a \left[\rho(x) A\left(\frac{\partial u(x,t)}{\partial t}\right)^2 - \mu(x) \frac{\partial}{\partial x} \left(\rho(x) A\frac{\partial u(x,t)}{\partial t}\right) \frac{\partial^2 u(x,t)}{\partial x \partial t} - E(x) A\left(\frac{\partial u(x,t)}{\partial x}\right)^2 \right].$$
(7)

2.3. Functionally graded materials

Functionally graded materials consist of at least two different materials. Variation of the material properties (elasticity modulus, density and nonlocal parameters) in the functionally graded structure are assumed in the exponential and power-law forms in the present study:

$$\begin{bmatrix} E(x)\\ \rho(x)\\ \mu(x) \end{bmatrix} = \begin{bmatrix} E_0\\ \rho_0\\ \mu_0 \end{bmatrix} e^{\lambda x} , \qquad (8)$$

$$\begin{bmatrix} E(x)\\ \rho(x)\\ \mu(x) \end{bmatrix} = \begin{bmatrix} E_1 - E_0\\ \rho_1 - \rho_0\\ \mu_1 - \mu_0 \end{bmatrix} x^y + \begin{bmatrix} E_0\\ \rho_0\\ \mu_0 \end{bmatrix} , \quad \begin{bmatrix} E_1\\ \rho_1\\ \mu_1 \end{bmatrix} = \begin{bmatrix} E_0\\ \rho_0\\ \mu_0 \end{bmatrix} s .$$
(9)

Equation (8) defines the exponential material variation, and Eq. (9) defines the power-law material variation in the CNT. In Eq. (8), λ is the material gradient index, and in Eq. (9), E_0 , ρ_0 , μ_0 and E_1 , ρ_1 , μ_1 are the material properties on the left and right side of the CNT; y is the power-law parameter, and s is the material coefficient.

2.4. The Ritz method

Axially graded rod structures have a governing equation of motion, which is a partial differential equation with variable material properties. A closed form solution of these types of differential equations cannot be obtained due to the variable coefficients. An approximate variational Ritz method can be used [9,10] in these instances. The longitudinal displacement function that is employed in the Ritz method is defined below with the assumption of the harmonic wave function $(u(x,t) = U(x)e^{-j\omega t})$ [11,12]:

$$U(x) = \sum_{m=m_0}^{J} \mathcal{C}_m \varphi_m(x), \tag{10}$$

where C_m are the unknown coefficients of the polynomial, and $\varphi_m(x)$ is the polynomial that satisfies at least the periodicity condition. $\varphi_m(\bar{x})$ is assumed to be in the Taylor series form and defined as follows:

$$\varphi_m(x) = \sum_{m=0}^J C_m \frac{x^m}{m!}.$$
(11)

To determine the longitudinal wave frequency of the CNT, the Lagrangian energy functional of the nanorod in Eq. (7) should be minimized with respect to unknown coefficients $\left(\frac{\partial L}{\partial C_m}\right)$.

3. Numerical results

The longitudinal wave propagation frequency of axially graded CNTs was investigated in this section. The effect of material gradient parameters on the wave propagation frequency of a nanotube was studied. The material property parameters of the CNT were assumed in a non-dimensional form. Numerical results were obtained in four different case studies: local non-grading, local grading, non-grading nonlocality, and grading nonlocality.

Three different solution methods were used in the analysis. First, the analytical solution was obtained for the exponential material variation in the non-grading nonlocality case. In the grading nonlocality case, a closed-form solution could not be obtained because of the variable nonlocal parameter in the inertia terms. The second and third methods were the higher order Haar wavelet method (HOHWM) [13] and the Ritz method, which were compared with the analytical results for validation. The HOHWM has become very popular in recent years and has been used in the static and dynamic analyses of nanostructures in several papers [14–18].

In Table 1, the longitudinal wave propagation frequencies at the end of the first Brillouin zone for different solution methods are presented. In the non-grading case, all solution methods give the same result. In the grading case, the analytical and HOHWM results coincide, but the Ritz method differs by a small percentage (<1%).

In Table 2, the convergence rates (Eq. (12)) of the HOHWM and Ritz methods are compared in exponentially non-grading and grading nonlocality cases. The *J* parameter is defined as the number

Table 1. Comparison of the solution methods

		Non-grading $(\lambda = 0)$)	Exponential grading ($\lambda = 1$)			
	Analytical	HOHWM $(J = 6)$	Ritz $(J = 6)$	Analytical	HOHWM $(J = 6)$	Ritz $(J=6)$	
$\mu = 0$	3.1416	3.1416	3.1416	3.1802	3.1802	3.1812	
$\mu = 0.01$	2.9972	2.9972	2.9972	3.0577	3.0577	3.0311	

Table 2. Exponentially graded CNTs: frequencies and convergence rates

J	$\lambda = 1, \mu = 0.01$				$\lambda=1,\mu_0=0.01$			
	HOHWM		Ritz		HOHWM		Ritz	
	Freq.	Conv. rate	Freq.	Conv. rate	Freq.	Conv. rate	Freq.	Conv. rate
2	3.05783	4.0298	3.34591	7.4776	2.99491	11.0957	3.19551	8.6295
3	3.05773	4.0079	3.29169	2.2392	2.99465	2.4115	3.17583	3.5792
4	3.05772	4.0020	3.03570	5.9864	2.99460	2.1089	2.94066	7.5699
5	3.05772	4.0005	3.03166	2.8859	2.99459	2.0234	2.93942	1.3607
6	3.05772	4.0001	3.03111	5.5433	2.99459	2.0034	2.93894	7.9056

of grid points in the CNT. The Ritz method shows good agreement with the HOHWM results, differing only by a small percentage. In the non-grading nonlocality case, HOHWM gives the fourth order convergence, which is normally expected. In the grading nonlocality case, the convergence rate drops to second order. The Ritz method could not achieve a certain convergence rate in non-grading and grading nonlocality cases. Still, the frequency results of the HOHWM and Ritz methods are close to each other.

Convergence rate =
$$\frac{\left|\frac{\omega_{J-1}-\omega_{J}}{\omega_{J}-\omega_{J+1}}\right|}{\log 2} .$$
(12)

In Table 3, the convergence rates for power-law grading can be seen. The difference between the HOHWM and Ritz methods increases slightly according to exponential grading. The difference in the frequency values increases to approximately 3% in the power-law variation. HOHWM approaches second-order convergence except in the weakened grading case (s = 0.5). The characteristics of the power-law variation are more effective than those of the exponential variation on the convergence rate.

According to Tables 2 and 3, the convergence rates in the HOHWM approach 4 or 2, depending on the grading nonlocality, whereas the convergence rates of the Ritz method vary. This shows the significant difference between the strong and weak formulation solutions.

Figure 1 shows the longitudinal wave propagation frequency variation of the CNT, which has exponentially grading material properties. The wave frequency characteristics mostly coincide in the HOHWM and Ritz methods. Enhancing material properties increases the frequency, while nonlocality decreases it. Grading nonlocality brings an additional softening effect on the structure, and frequency decreases.

Table 3. Power-law graded CNTs: frequencies and convergence rates

J	$S = 2, y = 2, \mu = 0.01$				$S = 2, y = 2, \mu_0 = 0.01$			
	HOHWM		Ritz		HOHWM		Ritz	
	Freq.	Conv. rate	Freq.	Conv. rate	Freq.	Conv. rate	Freq.	Conv. rate
2	3.04147	4.5281	3.26866	8.0416	3.01480	10.4190	3.20070	8.8331
3	3.04139	14.5169	3.23594	3.1105	3.01455	2.0995	3.18399	4.0053
4	3.04139	1.9880	2.95338	6.3872	3.01450	2.0149	2.91566	7.2986
5	3.04139	1.9995	2.95001	1.7880	3.01449	2.0022	2.91396	1.0231
6	3.04139	2.0013	2.94903	4.7239	3.01449	2.0000	2.91312	5.4293





Fig. 1. Wave frequency variation in exponentially grading material.



Fig. 2. Wave frequency variation in power-law material grading.

In Fig. 2, the effect of power-law material grading on the wave frequency can be seen. Similarly with the exponential material grading, grading nonlocality decreases the wave frequency. Conversely, the Ritz method shows a softening effect on the frequency without the nonlocal effect in the material grading cases.

4. Conclusion

Longitudinal wave propagation in axially graded carbon nanotubes was studied in the present work. Variations of material properties were assumed in exponential and power-law forms. The wave frequency was obtained using the analytical, higher order Haar wavelet and Ritz methods. The effects of material gradient parameters and grading nonlocality on the wave response of the axially graded carbon nanotube were investigated. As a novel approach, wave propagation was solved using weak energy formulation and the Ritz method. The results were compared and validated against closed and strong-form solutions. The present study could be useful in the wave dynamic analysis of axially graded nanostructures.

Data availability statement

All research data are contained within the article and can be shared upon request from the authors.

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Ritzi meetod teljesihis funktsionaalselt gradueeritud süsiniknanotorude lainelevi analüüsiks

Mustafa Arda ja Tamer Tosun

Töös on uuritud teljesihis funktsionaalselt gradueeritud süsiniknanotorude pikilainete levikut, rakendades kolme lahendusmeetodit: analüütilist meetodit, kõrgemat järku Haari lainikuid ja Ritzi meetodit. Erinevate meetoditega saadud tulemusi on võrreldud ja analüüsitud. Lagrange'i energia funktsionaali ja Ritzi meetodi abil on tuletatud nõrgal formulatsioonil põhinev lahendusmeetod laine sageduse määramiseks. Rakendatud on nii eksponentsiaalseid kui ka astmelisi gradueerimisfunktsioone. Uuritud on materjali gradueerimispara-meetrite ja mittelokaalsete efektide mõju pikilaine sagedusele. Töö pakub uusi võimalusi teljesihis gradueeritud nanostruktuuride lainedünaamika analüüsiks.