RESEARCH ARTICLE

Flexure mechanics of nonlocal modified gradient nano-beams

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Abstract

Two frameworks of the nonlocal integral elasticity and the modified strain gradient theory are consistently merged to conceive the nonlocal modified gradient theory. The established augmented continuum theory is applied to a Timoshenko–Ehrenfest beam model. Nanoscopic effects of the dilatation, the deviatoric stretch, and the symmetric rotation gradients together with the nonlocality are suitably accommodated. The integral convolutions of the constitutive law are restored with the equivalent differential model subject to the nonclassical boundary conditions. Both the elastostatic and elastodynamic flexural responses of the nano-sized beam are rigorously investigated and the well posedness of the nonlocal modified gradient problems on bounded structural domains is confirmed. The analytical solution of the phase velocity of flexural waves and the deflection and the rotation fields of the nano-beam is detected and numerically illustrated. The transverse wave propagation in carbon nanotubes is furthermore reconstructed and validated by the molecular dynamics simulation data. Being accomplished in revealing both the stiffening and softening structural responses at nano-scale, the proposed nonlocal modified gradient theory can be beneficially implemented for nanoscopic examination of the static and dynamic behaviors of stubby nano-sized elastic beams.

Keywords: Timoshenko–Ehrenfest beam; flexure; nonlocal integral elasticity; modified strain gradient theory; transverse wave propagation; nonclassical boundary conditions

1. Introduction

The vast implementation of nano-devices in modern engineering has stimulated a great deal of research on nano-mechanics (Nadeem et al., 2019; Mburu et al., 2021; Mondal & Pal, 2020; Rysaeva et al., 2020). As fundamental blocks of pioneering nanoelectromechanical systems viz. nano-resonators (Dilena et al., 2020; Sedighi & Ouakad, 2020) and nano-actuators (Ouakad et al., 2020; Sedighi et al., 2020a), nano-sized structures demonstrate peculiar size-dependent response that cannot be described via the traditional framework of the continuum mechanics. A variety of augmented continuum theories have thus emerged in the recent literature generally fallen under the classes of nonlocal continua, strain gradient continua, or nonlocal gradient continua (Shaat et al., 2020). In the context of the nonlocal elasticity, the nonlocal field at a point is defined as a weighted mean value in terms of the local field measured at the other points within the domain occupied by the continuum (Eringen, 2002). Reinstating the integral convolution of the nonlocal constitutive law with the differential relation yields paradoxical results as applied to nano-structures of applicative interest (Fuschi et al., 2019; Pisano et al., 2020). Contributions of either the surface elasticity (Zhu & Li, 2019; Li et al., 2020) or the higher order gradient theory (Faghidian, 2020a, b, c) to the nonlocal theory can beneficially overcome such anomalies. The recent literature amounts to a huge
contribution to the nonlocal elasticity model predicting a softening response in the mechanical behavior of nano-structures (Balbaid et al., 2019; Berghouti et al., 2019; Boutaleb et al., 2019; Hussain et al., 2019; Ansari et al., 2020; Asghar et al., 2020; Bel-lal et al., 2020; Elishakoff et al., 2020; Jena et al., 2020a, b; Rouabhia et al., 2020; Sedighi et al., 2020b; Shodja & Moosavian, 2020; Storch & Elishakoff, 2021). Alternatively, the main postulate governing the gradient elasticity indicates that the gradient field at a point depends not only on the classical kinematic field but also on the gradients of various orders. The higher order derivatives of the strain field are consequently assumed to affect the elastic strain energy (Mindlin, 1965). The modified strain gradient theory, accordingly, comprises additional dilatation gradient tensor, the deviatoric stretch gradient tensor, and the symmetric rotation gradient tensor compared to the classical elasticity approach (Lam et al., 2003). The stiffening structural response can be effectively realized consistent with the modified strain gradient theory as evidenced in the following representative works (Barretta et al., 2019a; Chayesh 2019a, b; Rouhi et al., 2019; Biash & Civalek, 2020; Civalek & Avcar, 2020; Soltani et al., 2021).

Since nano-structures may exhibit both the stiffening and softening behaviors, the nonlocal elasticity model and the modified strain gradient theory cannot solely represent the entire wide spectrum of the size-dependent phenomena at nano-scale (Wheel et al., 2015; Pisano et al., 2021). The unification of the nonlocal theory and the simplified strain gradient model is accordingly introduced in the literature (Aifantis, 2003; Polizzotto, 2015a). While the constitutive law of the nonlocal strain gradient model can be constructed by combining the pertinent constitutive equations of the augmented continuum theories, opting for the appropriate form of the nonclassical boundary conditions is still a matter of dispute (Zaera et al., 2019, 2020; Xu, 2021). The nonlocal strain gradient theory is being currently applied in a large number of researches (see e.g. Jalaei & Civalek, 2019; Barretta et al., 2019b, 2020a, b; Karami et al., 2019a, b; Tang et al., 2019; Jena et al., 2020c; Malikan & Eremeyev, 2020; Malikan et al., 2020; She, 2020; She et al., 2021; Torabi et al., 2020). The higher order kinematics effects, attributable to the modified strain gradient theory, cannot be realized in the framework of the nonlocal strain gradient theory and, accordingly, the nonlocal modified gradient theory is established in this study with application to Timoshenko–Ehrenfest nano-beams in flexure. In comparison with former studies, mostly investigating the nonlocal strain gradient model, the nano-scale effects of the dilatation gradient, the deviatoric stretch gradient, and the symmetric rotation gradient tensors along with the nonlocality are suitably taken into account. Furthermore, effects of shear deformation and rotary inertia are properly considered for stubby nano-sized beams. The modified strain gradient formulation of nano-beams is recalled in Section 2 and suitable forms of the higher order stress resultants and the higher order boundary conditions are introduced. The nonlocal elasticity theory in the original integral-type framework is unified with the modified strain gradient theory via a consistent variational approach in Section 3. Founded on suitable elastic functional, the integral convolutions of the stress resultants consistent with the nonlocal modified gradient theory are introduced and substituted with the equivalent differential constitutive model subject to nonclassical boundary conditions. The proposed constitutive model of the nonlocal modified gradient beam is demonstrated to be capable of capturing both the higher order gradients and the nonlocality effects. Sections 4 and 5 are, respectively, devoted to rigorously examine the elastodynamic and elastostatic responses of the Timoshenko–Ehrenfest nano-beam. Transverse wave propagation response is analytically examined and associated numerical results are elucidated and summarized. The elastostatic flexural response of stubby nano-beams for structural schemes of applicative interest, i.e. simply supported, cantilever, and fixed-end beams, is furthermore examined, graphically illustrated, and discussed. The conceived nonlocal modified gradient theory and associated analytical solutions for the elastic flexure of nano-beams can efficiently serve as the fundamental step toward developing computational methods (Anitescu et al., 2019; Guo et al., 2019; Samaniego et al., 2020) with a wider application spectrum in nano-mechanics. Conclusions are lastly outlined in Section 6.

2. Modified Strain Gradient Theory

To evoke the modified strain gradient mechanics of stubby beams, reference is made to a straight elastic beam of length L, referred to the Cartesian coordinate systems (x, y, z) as x, y, and z axes, respectively, coincide with the beam longitudinal axis, the beam width, and the height direction. The displacement field of a stubby beam, consistent with the Timoshenko–Ehrenfest beam model, can be expressed by (Polizzotto, 2015b; Faghidian, 2016; Elishakoff, 2019)

\[ u_1 = -z\psi(x, t), \quad u_2 = 0, \quad u_3 = w(x, t) \] (1)

with \( \psi \) and \( w \) being the cross-sectional rotation and the transverse displacement of the beam, respectively. In the framework of the modified strain gradient theory, additional material length-scale parameters \( \ell_0, \ell_1, \) and \( \ell_2 \) are introduced to, respectively, characterize the dilatation gradients, deviatoric stretch gradients, and symmetric rotation gradients (Lam et al., 2003). For ad hoc value of the gradient length-scale parameter \( \ell_2^4 = 16/\ell_1^2/15, \) the total elastic potential energy \( F \) and the kinetic energy \( K \) of the Timoshenko–Ehrenfest beam model are given by (Wang et al., 2015; Asghar et al., 2021)

\[ F = \int_0^L \left[ \frac{1}{2} D_1 (\partial_x \psi(x, t))^2 + \frac{1}{2} D_2 (\partial_x \psi(x, t))^2 \right. \]

\[ \left. + \frac{1}{2} D_1 (\partial_x w(x, t) - \psi(x, t))^2 + \frac{1}{2} D_2 (\partial_x w(x, t) - \partial_x \psi(x, t))^2 \right] \partial_x f(x, w(x, t)) \text{d}x \]

\[ K = \int_0^L \left[ \frac{1}{2} \rho A (\partial_x w(x, t))^2 + \frac{1}{2} \rho I (\partial_x \psi(x, t))^2 \right] \text{d}x, \] (2)

where \( \rho \) denotes the material density along with \( A \) and \( I, \) respectively, representing the cross-sectional area and the second moment of area about the y-axis. The stubby beam is assumed to be subjected to a distributed transverse loading \( f. \) The so-called higher order flexural stiffness parameters \( D_1, D_2 \) and the shear stiffness parameters \( B_1, B_2 \) are also introduced as (Wang et al., 2010)

\[ D_1 = EI + GA \left( 2\ell_0^2 + \frac{8}{5} \ell_1^2 \right), \quad D_2 = GI \left( 2\ell_0^2 + \frac{4}{5} \ell_1^2 \right) \]

\[ B_1 = kGA, \quad B_2 = \frac{4}{5} \ell_1^2 GA \] (3)

with \( E \) and \( G \) correspondingly designating the elastic and shear moduli and \( k \) stands for the shear correction factor (Kaneko, 1978; Bourada et al., 2020; Bousahla et al., 2020; Matouk et al., 2020). Performing the first-order variation of the Lagrangian...
functional $L = k - f$, followed by integration by parts, leads to

$$
\tilde{s}_L = \int_0^L \left[ D_1 \partial_{xx} \psi (x, t) \right. \left. - D_2 \partial_{xxx} \psi (x, t) + B_1 (\partial_w w (x, t) - \psi (x, t)) \right. \left. - B_2 (\partial_{xxw} w (x, t) - \partial_{xw} \psi (x, t)) \right] d\bar{x}
$$

$$
+ \left[ B_1 (\partial_{xxw} w (x, t) - \partial_{xw} \psi (x, t)) - B_2 (\partial_{xxx} \psi (x, t)) \right.
$$

$$
= -B_2 \left( \partial_{xxw} w (x, t) - \partial_{xw} \psi (x, t) \right) d\bar{x} + \left( -D_1 \partial_{xw} \psi + D_2 \partial_{xxx} \psi \right) \delta \psi \big|_0^L
$$

$$
- \left( B_1 (\partial_w w - \psi) - B_2 (\partial_{xxw} w - \partial_{xw} \psi) \right) \delta w \big|_0^L
$$

$$
- \left( D_2 \partial_{xxx} \psi \right) \big|_0^L - B_2 (\partial_{xxx} \psi - \partial_{xxw} w) \big|_0^L = 0.
$$

(4)

With regard to the detected variation of the Lagrangian functional, the flexural moment $M$ and the shear force $V$ associated with the modified strain gradient Timoshenko–Ehrenfest beam are, respectively, introduced by

$$
M (x, t) = -D_1 \partial_w w (x, t) + D_2 \partial_{xxw} \psi (x, t)
$$

$$
= -D_1 \partial_w w (x, t) + D_2 \partial_{xxw} \psi (x, t)
$$

$$
V (x, t) = B_1 (\partial_w w (x, t) - \psi (x, t)) - B_2 (\partial_{xxw} w (x, t) - \partial_{xw} \psi (x, t))
$$

$$
= B_1 (\partial_w w (x, t) - \psi (x, t)) - B_2 (\partial_{xxw} w (x, t) - \partial_{xw} \psi (x, t)).
$$

(5)

The constitutive laws of the stress resultant fields $M, V$ are properly defined in terms of the flexural curvature $k = \partial_w \psi$ and the shear strain field $\gamma = \partial_{xx} w - \psi$ and of their second-order gradients. The classical constitutive model of the Timoshenko–Ehrenfest beam can be noticeably obtained via vanishing of the gradient length-scale parameters. The differential and boundary conditions of dynamic equilibrium of a Timoshenko–Ehrenfest beam consistent with the modified strain gradient theory can be thus determined, while assuming arbitrary variations of the flexural curvature and the shear strain fields,

$$
-\partial_t M (x, t) + V (x, t) = \rho \partial_t \psi (x, t)
$$

$$
\partial_t V (x, t) + f (x) = \rho \partial_t \partial_w w (x, t)
$$

$$
M \delta \psi \big|_0^L = V \delta w \big|_0^L = 0
$$

$$
(D_2 \partial_{xxx} \psi) \big|_0^L = (B_2 \partial_{xw} \gamma) \big|_0^L = 0.
$$

(6)

Not only the constitutive laws of the modified strain gradient stubby nano-beam are suitably introduced via the proposed variational framework, but also the differential and boundary conditions of dynamic equilibrium along with the higher order boundary conditions are aptly reestablished.

3. Nonlocal Modified Gradient Theory

The nonlocality contribution can be appropriately introduced to the modified strain gradient theory in the framework of the nonlocal modified gradient theory implementing the elastic variational functional $L$ defined as

$$
E = \frac{1}{2} D_1 \int_0^L \int_0^L \left[ k (x, \xi) \alpha (x - \bar{x}, \xi) \psi (x, t) \right] d\bar{x} d\xi
$$

$$
+ \frac{1}{2} D_2 \int_0^L \int_0^L \left[ \partial_{xx} \psi (x, t) \right. \left. - \partial_{xw} \psi (x, t) \right] d\bar{x} d\xi
$$

$$
+ \frac{1}{2} B_1 \int_0^L \int_0^L \left[ \gamma (x, \xi) \alpha (x - \bar{x}, \xi) \gamma (x, t) \right] d\bar{x} d\xi
$$

$$
+ \frac{1}{2} B_2 \int_0^L \int_0^L \left[ \partial_{xw} \gamma (x, \xi) \alpha (x - \bar{x}, \xi) \partial_{xw} \gamma (x, t) \right] d\bar{x} d\xi.
$$

(7)

with $x, \bar{x}$ being the points of the beam domain. The averaging nonlocal kernel $\alpha$ is enriched with the nonlocal length-scale parameter $c$ and supposed to meet the necessary properties of positivity, symmetry, normalization, and limit impulsivity (Romano & Diaco, 2021).

To formulate the constitutive model of the stress resultant fields $M, V$ consistent with the nonlocal modified gradient theory, directional derivatives of the elastic variational functional along a virtual curvature and a virtual shear strain, having compact support in the beam domain, are first evaluated. Setting equal the achieved results to the virtual work associated with the Timoshenko–Ehrenfest nano-beam, for arbitrary choices of the virtual kinematic fields, yields

$$
M (x, t) = -D_1 \int_0^L \alpha (x - \bar{x}, \xi) \psi (x, t) \bar{\delta} \psi d\bar{\xi}
$$

$$
+ D_2 \partial_{xxw} \psi \int_0^L \alpha (x - \bar{x}, \xi) \partial_{xw} \gamma (x, t) \bar{\delta} \gamma d\bar{\xi}
$$

$$
V (x, t) = B_1 \int_0^L \alpha (x - \bar{x}, \xi) \psi (x, t) \bar{\delta} \psi d\bar{\xi}
$$

$$
- B_2 \partial_{xxw} \psi \int_0^L \alpha (x - \bar{x}, \xi) \partial_{xw} \gamma (x, t) \bar{\delta} \gamma d\bar{\xi}.
$$

(8)

To determine the differential constitutive laws, equivalent to the introduced integral convolutions, the averaging nonlocal kernel $\alpha$ is assumed to coincide with the bi-exponential kernel function, a well-recognized kernel frequently adopted in the nonlocal theory (Romano & Diaco, 2021),

$$
\alpha (x, c) = \frac{1}{2c} \exp \left( -\frac{|x|}{c} \right).
$$

(9)

The nonlocal modified gradient constitutive model equation (8), enriched with the bi-exponential kernel function equation (9), can be consistently replaced with the differential constitutive relations. In the framework of the nonlocal modified gradient theory, the equivalent differential formulation of the flexural moment $M$ and the associated nonclassical boundary conditions are accordingly determined as

$$
\frac{1}{c^2} \partial_t M (x, t) - \partial_{xx} M (x, t) = -D_1 \frac{1}{c^2} \left[ \partial_t \psi (x, t) + \frac{D_2}{c^2} \partial_{xxw} \psi (x, t) \right]
$$

$$
\partial_t \partial_{xxw} w (0, t) = \frac{1}{c \partial_t \psi (0, t)} - \frac{D_2}{c^2} \partial_{xxw} \psi (0, t)
$$

$$
\partial_t \partial_{xxw} \psi (L, t) + \frac{1}{c \partial_t \psi (L, t)} = \frac{D_2}{c^2} \partial_{xxw} \psi (L, t).
$$

(10)

Likewise, the equivalent differential law of the shear force $V$ and the corresponding nonclassical boundary conditions are established as

$$
\frac{1}{c^2} \partial_t V (x, t) - \partial_{xx} V (x, t) = \frac{B_1}{c^2} \gamma (x, t) + \frac{B_2}{c^2} \partial_{xxw} w (x, t)
$$

$$
\partial_t \partial_{xxw} w (0, t) = \frac{B_1}{c \partial_t \gamma (0, t)} - \frac{B_2}{c^2} \partial_{xxw} \psi (0, t)
$$

$$
\partial_t \partial_{xxw} \psi (L, t) + \frac{1}{c \partial_t \gamma (L, t)} = \frac{B_2}{c^2} \partial_{xxw} \psi (L, t).
$$

(11)

To achieve the closure of the differential constitutive problem on bounded domains of nano-mechanics interest, the introduced nonclassical boundary conditions should be properly imposed. The stress resultants as the solution of the integral convolutions of the constitutive model can be demonstrated to effectively fulfill the equilibrium conditions, in view of rigorous
examination of the elastostatic flexure response presented in Section 5. The equivalence of the conceived integral convolutions to the differential constitutive relation is therefore assured. In consideration of the limit impulsivity property of the nonlocal kernel, i.e. \( \lim_{c \to 0} a(x, c) = \delta(x) \) with \( \delta \) representing the Dirac unit impulse, the constitutive laws of the modified strain gradient stubby beam and associated higher order boundary conditions can be reestablished (Wang et al., 2010):

\[
M(x, t) = -D_1 \partial_x^2 M(x, t) + D_2 \partial_x^4 M(x, t) \\
V(x, t) = B_1 \partial_x^2 V(x, t) - B_2 \partial_x^4 V(x, t) \\
\partial_x \partial_x M(0, t) = \partial_x \partial_x M(L, t) = 0 \\
B_2 \partial_x V(0, t) = B_2 \partial_x V(L, t) = 0.
\]

Setting the higher order flexural stiffness parameters \( D_1 = \ell_s^4 D_1 = \ell_s^2 E I \) and the shear stiffness parameters \( B_2 = \ell_s^4 B_1 = \ell_s^2 k G A \), the constitutive law of the Timoshenko–Ehrenfest beam and the corresponding nonclassical boundary conditions consistent with the nonlocal strain gradient model can be furthermore obtained as a particular case of the conceived size-dependent elasticity theory (Barretta et al., 2019b):

\[
\frac{1}{c^2} M(x, t) - \partial_x M(x, t) = -\frac{E I}{c^2} \partial_x^2 (x, t) + \frac{E I \ell_s^2}{c^2} \partial_x^4 (x, t) \\
\frac{1}{c^2} V(x, t) - \partial_x V(x, t) = \frac{k G A}{c^2} \partial_x^2 (x, t) - \frac{k G A}{c^2} \partial_x^4 (x, t) \\
\partial_x M(0, t) - \frac{1}{c} M(0, t) = -\frac{E I \ell_s^2}{c^2} \partial_x^2 (0, t) \\
\partial_x M(L, t) + \frac{1}{c} M(L, t) = -\frac{E I \ell_s^2}{c^2} \partial_x^2 (L, t) \\
\partial_x V(0, t) - \frac{1}{c} V(0, t) = \frac{k G A}{c^2} \partial_x^2 (0, t) \\
\partial_x V(L, t) + \frac{1}{c} V(L, t) = \frac{k G A}{c^2} \partial_x^2 (L, t).
\]

where \( \ell_s \) denotes the gradient length-scale parameter associated with the simplified strain gradient theory demonstrating the significance of the first-order strain gradient field. The nonlocal strain gradient model and the established nonlocal modified gradient theory are strictly related to the same governing differential and boundary conditions but equipped with dissimilar higher order stiffness parameters. The nonlocal strain gradient model has been thus considered apposite for comparison with the nonlocal modified gradient theory.

4. Wave Propagation Analysis

The wave propagation phenomenon is well established to be considerably affected by the nano-structural features of materials. The classical continuum theory fails in appropriate prediction of the wave response particularly for wavelengths at nano-scale. Appropriate description of the dispersive behavior of waves is the main focus of recent researches via implementing a range of augmented continuum theories (see e.g. de Domenico et al., 2018, 2019; Shodja & Moosavian, 2020).

To study the propagation behavior of flexural waves, the Timoshenko–Ehrenfest beam model in the framework of the nonlocal modified gradient theory is considered. In view of the differential equations of dynamic equilibrium (6), (12) and the established constitutive law equations (10), (11), the flexural moment \( M \) and the shear force \( V \) are, respectively, determined as

\[
M(x, t) = c^2 \rho A \partial_x w(x, t) - c^2 \rho I \partial_x^2 \psi(x, t) \\
- D_2 \partial_x \psi(x, t) + D_2 \partial_x \psi(x, t) \\
V(x, t) = c^2 \rho A \partial_x w(x, t) + B_1 (\partial_x w(x, t) - \psi(x, t)) \\
- B_2 (\partial_x w(x, t) - \partial_x \psi(x, t)).
\]

where the distributed transverse load is overlooked in the elastodynamic analysis. By substitution of the stress resultant fields \( M, V \) into the differential conditions of dynamic equilibrium, a set of governing equations for the Timoshenko–Ehrenfest beam is obtained as

\[
c^2 \rho I \partial_x^2 \psi(x, t) + D_1 \partial_x \psi(x, t) - D_2 \partial_x \psi(x, t) \\
+ B_1 (\partial_x \psi(x, t) - \psi(x, t)) - B_2 (\partial_x^2 \psi(x, t) - \partial_x \psi(x, t)) \\
- \rho I \partial_t \psi(x, t) = 0 \\
c^2 \rho A \partial_x w(x, t) + B_1 (\partial_x w(x, t) - \partial_x \psi(x, t)) \\
- B_2 (\partial_x^2 w(x, t) - \partial_x \psi(x, t)) - \rho A \partial_t w(x, t) = 0.
\]

Upon substitution of the pertinent higher order stiffness parameters, the aforementioned governing equations are identical to those obtained in Wu et al. (2013) for the Timoshenko–Ehrenfest beam consistent with the nonlocal strain gradient model. For slowly varying fields defined on unbounded domains, the condition of decay at infinity holds and, accordingly, the nonclassical boundary conditions can be released. For transverse waves propagating in nano-beams, a proper analytical solution can be thus expressed as

\[
\psi(x, t) = \Psi \exp \left( i \lambda (x - C_p t) \right), w(x, t) = W \exp \left( i \lambda (x - C_p t) \right),
\]

where \( \Psi \) and \( W \) are the coefficients of the wave amplitudes along with \( \lambda \) and \( C_p \), respectively, denoting the wave number and the phase velocity. Prescribing the wave propagation solution equation (16) into the governing equations (15) results in a homogeneous set of algebraic equations that should be singular in order to have a nontrivial solution. The characteristic equation of the flexural wave propagation is therefore detected via vanishing of the determinant of coefficients of the homogeneous algebraic system as

\[
-\epsilon^4 (1 + \epsilon^4) \rho^2 A + C_p^2 \lambda^2 (1 + \epsilon^4) (B_1 (\rho A + \lambda^2 \rho I)) \\
+ \lambda^2 ((D_1 + D_2 \lambda^2) \rho A + B_2 (\rho A + \lambda^2 \rho I))) \\
- \lambda^4 (B_1 + B_2 \lambda^2) (D_1 + D_2 \lambda^2) = 0.
\]

There exist two positive roots for each wave number and, accordingly, transverse waves have two branches where the lower branch corresponds to the flexural wave. A comparison of the phase velocity of flexural waves provided for the Timoshenko–Ehrenfest beam based on the nonlocal strain gradient model and the nonlocal modified gradient theory is made in Fig. 1. The illustration is furthermore enriched by demonstrating the wave propagation results detected via the molecular dynamics (MD) simulation for (5.5) armchair carbon nanotube (Wang & Hu, 2005). The material length-scale parameters of the augmented continuum theories are determined by applying the inverse theory approach (Farahni et al., 2009, 2010) while utilizing the mechanical properties of the (5.5) armchair carbon nanotube (de Domenico & Askes, 2018; Khorshidi, 2020). To reduce the influence of the uncertainty in measurements and to assure the continuous dependence of the reconstructed results on the simulation data, either frameworks of the
regularization theory (Faghidian, 2014, 2015) or the probabilistic sensitivity analysis (Vu-Bac et al., 2016) can be furthermore implemented. The identified characteristic parameters are collected in Table 1.

As deducible from the illustrative results in Fig. 1, the phase velocity of wave propagation consistent with either of the augmented continuum theories is close to the MD simulations for small wave numbers, i.e. when the wave number \( \lambda \) is smaller than 3[1/nm]. With increasing the wave number, the discrepancy between the wave propagation results associated with the nonlocal strain gradient model and the nonlocal modified gradient theory is pronounced. The phase velocity consistent with the nonlocal modified gradient theory, nevertheless, agrees better with the simulation data as the wave number rises. The nanoscopic phenomenon can be practically clarified in view of the importance of nano-structural properties for only large wave numbers. It is of notice that the phase velocity of transverse waves is not sensitive to nano-material properties for low wave numbers. Indeed, the scaling effect on the wave propagation behavior is noteworthy once the wavelengths become small enough to be comparable with the length-scale parameters. The reliability of an augmented continuum theory in description of the wave propagation should be accordingly examined for large wave numbers. The importance of using the appropriate augmented continuum theory to properly describe the wave propagation phenomenon is therefore illustrated.

As the nonlocal strain gradient model and the nonlocal modified gradient theory are enriched with different numbers of the gradient length-scale parameters, a practical choice preferred in the literature is to assume \( c_0 = c_1 = \ell \) (Wang et al., 2010; Asghari et al., 2012). In the sequel, the acronyms LOC, NG, and NmodG, correspondingly, stand for the local beam model, nonlocal strain gradient model, and nonlocal modified gradient theory. To consistently investigate the size effects of the length-scale parameters on the phase velocity of flexural waves, the nondimensional parameters, namely radius of gyration \( \epsilon \), nonlocal characteristic parameter \( \zeta \), gradient characteristic parameters \( \eta, \eta_s \), wave number \( \lambda \), and phase velocity \( \bar{C}_p \), are, respectively, introduced as

\[
\bar{h} = \frac{1}{L} \sqrt{\frac{I}{A}}, \quad \zeta = \frac{\lambda}{L}, \quad \eta = \frac{\ell}{L}, \quad \eta_s = \frac{\ell_s}{L}, \quad \bar{\lambda} = \lambda L, \quad \text{and} \quad \bar{C}_p = \frac{C_p}{C_{p,\text{LOC}}} \sqrt{\frac{\rho A}{E I}}.
\]

The detected phase velocity of flexural waves is normalized with respect to the pertinent phase velocity of the local beam model \( \bar{C}_{p,\text{LOC}} \). 3D variation of the normalized phase velocity \( \bar{C}_p/C_{p,\text{LOC}} \) with respect to the logarithmic scaling of \( \bar{\lambda} \) (Caprio, 2005) is illustrated here for the nonlocal modified gradient theory in comparison with the nonlocal strain gradient model. Nanoscopic effects of the nonlocal and gradient characteristic parameters are correspondingly investigated in Figs 2 and 3. While the varying characteristic parameters are assumed to range in the interval \([0, 1]\), the (logarithm of) nondimensional wave number \( \bar{\lambda} \) is ranging in the interval \([10^0, 10^2]\). The nondimensional radius of gyration is prescribed as \( \bar{h} = 1/10 \).

Both the augmented continuum theories coincide in the absence of the gradient length-scale parameters, and thus, the effect of the nonlocal characteristic parameter on the propagation response of flexural waves is studied in Fig. 2 for equal nonvanishing values of the gradient parameters \( \eta = \eta_s = 1/2 \). The effect of the gradient characteristic parameter on the wave propagation phenomenon is examined in Fig. 3 for vanishing of the

| \( \bar{c} \)(nm) \ | \( \ell_0 \)(nm) \ | \( \ell_1 \)(nm) \ | \( \ell_2 \)(nm) |
|---|---|---|---|
| NmodG elasticity theory | 0.34068 | 0.11924 | 0.20207 | 0.20869 |
| NG elasticity theory | 0.48097 | 0.16784 | - | - |

Table 1: Length-scale parameter identification for (5, 5) carbon nanotube consistent with MD simulation data.
nonlocal length-scale parameter. As clearly observed in the numerical results, the nonlocal and gradient characteristic parameters have the effects of decreasing and increasing the phase velocity, respectively. A larger value of $\zeta$ and $\eta$, accordingly, involves a smaller and larger phase velocity. The softening and stiffening responses in terms of the nonlocal and gradient characteristic parameters are therefore revealed in either of frameworks of the augmented continuum theories. For low wave numbers, corresponding to high wavelengths, the flexural wave propagation response approaches the phase velocity results of the local beam model. The discrepancy between the numerical results of the phase velocity is merely enhanced at higher wave numbers noticeably demonstrating the sensitivity of the wave propagation phenomenon to the nano-material properties at lower wavelengths. Indeed, as the wavelength is small enough to be commensurate with the characteristic lengths, the nanoscopic effect on the phase velocity of wave propagation will become considerable. The phase velocity of wave propagation associated with the nonlocal strain gradient model is also detected to be considerable. The phase velocity of wave propagation associated with the nonlocal modified gradient theory in corporates additional degrees of freedom in the kinematics assumptions for each material point, and accordingly, will lead to more stiffening response compared with the nonlocal strain gradient model.

5. Flexure Analysis

The elastostatic flexural response of the Timoshenko–Ehrenfest beam in the framework of the nonlocal modified gradient theory is rigorously examined here and the analytical solution of the transverse displacement and the rotation fields of the nano-beam are derived. The nano-beam is assumed to be subjected to a uniformly distributed transverse load $f$. A set of governing equations of the Timoshenko–Ehrenfest beam in the absence of the inertial terms is recalled as

$$D T \partial_{xx} \psi (x) - D \partial_{xxx} \psi (x) + B_1 (\partial_{xx} w (x) - \psi (x)) - B_2 (\partial_{xxx} w (x) - \partial_{xx} \psi (x)) = 0$$

$$B_1 (\partial_{xx} w (x) - \partial_{xx} \psi (x)) = 0$$

The maximum transverse deflection of the nano-sized beam is also normalized with respect to the pertinent flexural response of the local beam model $w_{LOC}$, for the illustrative purpose. Nanoscopic effects of the characteristic parameters on the normalized maximum transverse displacement of the Timoshenko–Ehrenfest nano-beam are, respectively, examined in Figs 4–6 for simply supported, cantilever, and fixed-end boundary conditions. The characteristic parameters are supposed to have the same ranging interval as the wave propagation analysis, while the nondimensional radius of gyration is set to 1/10.

As inferred from 3D illustrations, increasing the nonlocal and gradient characteristic parameters, respectively, increases and

![Figure 4: Effects of characteristic parameters on the flexural response of a uniformly loaded simply supported nano-beam.](https://academic.oup.com/jcde/article/8/3/949/6279760)
Figure 5: Effects of characteristic parameters on the flexural response of a uniformly loaded cantilever nano-beam.

Figure 6: Effects of characteristic parameters on the flexural response of a uniformly loaded fixed-end nano-beam.

decreases the nondimensional transverse displacement of the nano-sized beam with respect to the local beam model. The nonlocal and gradient characteristic parameters have, correspondingly, the effect of softening and stiffening the flexural response of the nano-beam for both the augmented continuum theories. The flexural response of the Timoshenko–Ehrenfest beam consistent with the nonlocal strain gradient model is realized to be strictly higher than, and hence overestimates, the counterpart flexure results of the nonlocal modified gradient theory. In both frameworks of the nonlocal modified gradient theory and the nonlocal strain gradient model, the flexure response of the local elasticity model is therefore retrieved in the absence of the length-scale characteristic parameters. The normalized maximum deflections of the Timoshenko–Ehrenfest beam, determined consistent with the nonlocal strain gradient and the nonlocal modified gradient theories, are, respectively, collected in Tables 2–4 for simply supported, cantilever, and fixed-end boundary conditions.

Table 2: Normalized maximum transverse deflection of a simply supported nano-beam.

| ζ  | η = 0 | η = 0.2 | η = 0.4 | η = 0.6 | η = 0.8 | η = 1.0 | ζ  | η = 0 | η = 0.2 | η = 0.4 | η = 0.6 | η = 0.8 | η = 1.0 |
|----|------|--------|--------|--------|--------|--------|----|------|--------|--------|--------|--------|--------|
| 0  | 1.00000 | 0.83196 | 0.69433 | 0.63142 | 0.60133 | 0.58532 | 1.00000 | 0.29307 | 0.11975 | 0.06156 | 0.03672 | 0.02419 |
| 0.2| 1.61149 | 1.20695 | 0.88708 | 0.73887 | 0.66776 | 0.62990 | 1.61149 | 0.57516 | 0.25058 | 0.13086 | 0.07851 | 0.05186 |
| 0.4| 2.95141 | 1.91802 | 1.23266 | 0.92821 | 0.78402 | 0.70765 | 2.95141 | 1.05554 | 0.46630 | 0.24433 | 0.14677 | 0.09701 |
| 0.6| 5.01976 | 2.96518 | 1.73107 | 1.19947 | 0.95012 | 0.81857 | 5.01976 | 1.73420 | 0.76689 | 0.40197 | 0.24151 | 0.15963 |
| 0.8| 7.81655 | 4.34843 | 2.38232 | 1.55263 | 1.16605 | 0.96266 | 7.81655 | 2.61113 | 1.15237 | 0.60378 | 0.36271 | 0.23973 |
| 1.0| 11.34178 | 6.06775 | 3.18640 | 1.98769 | 1.43181 | 1.13993 | 11.34178 | 3.68634 | 1.62272 | 0.84976 | 0.51038 | 0.33730 |

6. Conclusions

The nonlocal modified gradient theory is conceived in this study via the consistent unification of the nonlocal integral elasticity and the modified strain gradient theory. In comparison with preceding contributions, mainly devoted to the nonlocal strain gradient model, nanoscopic effects of the dilatation gradient, the deviatoric stretch gradient, and the symmetric rotation gradient tensors in conjunction with the nonlocality are appropriately taken into consideration. The Timoshenko–Ehrenfest beam model is selected for the structural modeling that can properly take account of the shear deformation and the rotary inertia. The nonlocal elasticity model, simplified and modified strain gradient theory, and the nonlocal strain gradient theory are demonstrated to be reestablished under ad hoc assumptions.

The analytical solution of the phase velocity of wave propagation as well as the transverse deflection and rotation fields of the Timoshenko–Ehrenfest nano-beam is determined. The dispersive behavior of flexural waves in carbon nanotubes is reconstructed and confirmed by the MD data. The importance of applying the appropriate augmented continuum
Table 3: Normalized maximum transverse deflection of a cantilever nano-beam.

| ζ | NG elasticity theory | NmodG elasticity theory |
|---|----------------|-------------------------|
|   | η = 0 | η = 0.2 | η = 0.4 | η = 0.6 | η = 0.8 | η = 1.0 | η = 0 | η = 0.2 | η = 0.4 | η = 0.6 | η = 0.8 | η = 1.0 |
| 0° | 1.00000 | 0.13186 | 0.32664 | 0.77997 | 0.75695 | 0.74455 | 1.00000 | 0.27652 | 0.19052 | 0.17230 | 0.16572 | 0.16264 |
| 0.2 | 1.87202 | 1.04010 | 1.37833 | 1.26553 | 1.21011 | 1.18032 | 1.87202 | 0.44546 | 0.28294 | 0.24857 | 0.23618 | 0.23038 |
| 0.4 | 2.01575 | 1.04531 | 0.78731 | 0.26824 | 0.17971 | 0.19771 | 2.01575 | 1.41443 | 0.27399 | 0.16499 | 0.10917 |
| 0.6 | 4.42521 | 3.64651 | 2.74176 | 2.20760 | 2.11315 | 2.08332 | 4.42521 | 2.23464 | 0.74328 | 0.59480 | 0.54132 | 0.51628 |
| 0.8 | 6.10640 | 4.64098 | 3.55350 | 3.01563 | 2.75191 | 2.61022 | 6.10640 | 1.14850 | 0.61459 | 0.50207 | 0.46154 | 0.44256 |
| 1.0 | 8.05731 | 5.97983 | 4.45192 | 3.69678 | 3.32660 | 3.12772 | 8.05731 | 1.44826 | 0.74328 | 0.59480 | 0.54132 | 0.51628 |

Table 4: Normalized maximum transverse deflection of a fixed-end nano-beam.

| ζ | NG elasticity theory | NmodG elasticity theory |
|---|----------------|-------------------------|
|   | η = 0 | η = 0.2 | η = 0.4 | η = 0.6 | η = 0.8 | η = 1.0 | η = 0 | η = 0.2 | η = 0.4 | η = 0.6 | η = 0.8 | η = 1.0 |
| 0° | 1.00000 | 0.62430 | 0.31660 | 0.17594 | 0.10866 | 0.07287 | 1.00000 | 0.47618 | 0.21750 | 0.11479 | 0.06914 | 0.04575 |
| 0.2 | 2.72024 | 1.57616 | 0.78731 | 0.26824 | 0.17971 | 0.19771 | 2.72024 | 1.41443 | 0.27399 | 0.16499 | 0.10917 |
| 0.4 | 5.91217 | 3.64651 | 2.74176 | 2.20760 | 2.11315 | 2.08332 | 5.91217 | 2.23464 | 0.74328 | 0.59480 | 0.54132 | 0.51628 |
| 0.6 | 10.66141 | 6.51036 | 3.71045 | 1.48244 | 0.90960 | 0.60805 | 10.66141 | 3.76418 | 1.68243 | 0.88401 | 0.53161 | 0.35153 |
| 0.8 | 17.00086 | 8.73077 | 4.17624 | 2.27671 | 1.39508 | 0.93198 | 17.00086 | 5.73328 | 2.54652 | 1.33626 | 0.80319 | 0.53099 |
| 1.0 | 24.94589 | 12.59520 | 5.98113 | 3.25285 | 1.99125 | 1.32960 | 24.94589 | 8.43434 | 3.59981 | 1.88699 | 1.13378 | 0.74941 |

theory to accurately describe the wave propagation phenomenon is demonstrated. The elastostatic flexural response of stubby nano-beams for structural schemes of applicative interest is examined and discussed. The well posedness of the established nonlocal modified gradient problems on bounded structural domains is thus assured. The pronounced stiffening effect of the gradient characteristic parameters corresponding to the nonlocal modified gradient theory is confirmed. A consistent augmented continuum theory is conceived that can constructively describe the size effects in both the elastostatic and elastodynamic flexure of stubby nano-beams while noticeably being exempt from anomalies typical of the size-dependent formulations.

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Conflict of interest statement

None declared.

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