Nonlocal Gradient Approach on Torsional Vibration of CNTs

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Abstract

The nonlocal strain gradient approach for torsional vibration of CNTs have been investigated in the present study. The effects of the stress and strain gradient small scale parameters on the non-dimensional frequencies have been obtained. Strain Gradient Theory has stiffening effect on the dynamics of CNT. Combination of both theories gives more acceptable results according to Lattice Dynamics.

Key words: torsional vibration, carbon nanotubes, nonlocal gradient theory.

Нелокальный градиентный подход для крутильных колебаний УНТ

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Аннотация

В данном исследовании был рассмотрен подход нелокального градиента деформации для крутильных колебаний УНТ. Было определено влияние микропараметров градиента напряжения и деформации на безразмерных частотах. Теория градиента деформации имеет эффект повышения жесткости на динамику УНТ. Сочетание обеих теорий дает более приемлемые результаты в соответствии с динамикой решетки.

Ключевые слова: *Крутильные колебания, Углеродные нанотрубки, Теории нелокального градиента.*

Introduction

Nowadays, scientists and engineers have great interest on CNTs, which were discovered by Iijima [1] in 1991, because of CNTs' superior physical properties. Analysis related to circumferential direction in CNTs has gained importance especially in design process of nano-motors, nano-bearings and nano-gearboxes.

Classical theories couldn't be applied in nanoscale analysis because of their size independence. Nonlocal Theory, proposed by Eringen [2, 3], is a continuum theory and includes size dependence. Stress and strain gradient approaches can be applied with the nonlocal theory. These nonlocal gradient approaches give more acceptable results when compared to the classical theories. Eringen adjust the wave dispersion curves according to Lattice Dynamics and with this assumption Eringen combined continuum and discrete theories as one theory.

In literature search, lots of study can be found about nonlocal stress gradient theory, but application of nonlocal strain gradient theory can be seen barely. Wang and Varadan developed a nonlocal continuum mechanics model and applied to the both single-walled carbon nanotubes (SWCNTs) and double-walled carbon nanotubes (DWCNTs). They investigated the small-scale effects on vibration characteristics of CNTs [4]. Duan et al. adjusted the e_0 parameter for the Nonlocal Timoshenko Beam Theory in free vibration case of

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SWCNTs. They used vibration frequencies generated from Moleculer Dynamics (MD) Simulation for optimization of (e_0) parameter [5]. Kumar et al. studied the buckling of CNTs using nonlocal one dimensional Euler-Bernoulli Beam Model. They used both stress and strain gradient approach and variational principle in model and boundary conditions [6]. Lim applied the Nonlocal Elasticity Field Theory to nano-mechanics and variational principle. He derived the main governing equation and boundary conditions for bending case [7]. Şimşek studied the forced vibration of simply supported SWCNT under the moving harmonic load effect. He used the Nonlocal Euler-Bernoulli Beam Theory in modeling [8]. Zhang et al. developed a hybrid Nonlocal Euler–Bernoulli Beam Model for bending, buckling and vibration analysis of nanobeams. The strain energy functional combines the local and nonlocal curvatures in the hybrid model that has two independent small-length scale parameters unlike Eringen's Nonlocal Model [9]. Ansari et al. investigated the vibrational characteristic of SWCNTs based on the gradient elasticity theory. They applied different gradient elasticity theories like stress, strain and combined one to nanotube for showing the nonlocal effect [10]. Thai proposed a Nonlocal Shear Deformation Beam Theory for bending, buckling and vibration case using Eringen's nonlocal differential constitutive relations. He didn't use shear correction factor in his model that account for both small scale effects and quadratic variation of shear strain together [11]. Narendar et al. studied the torsional vibration of nanorods using Strain Gradient Theory which is a non-classical theory and includes size effect [12]. Wang developed two beam model for vibration analysis of fluid conveying nanotubes using strain gradient elasticity combined with inertia gradients [13]. Wang and Wang investigated the vibration of nanotubes embedded in an elastic matrix by using Nonlocal Timoshenko Beam Model. They considered both stress and strain gradient approaches in formulation [14]. Arda and Aydogdu made the static and dynamic analysis of CNTs embedded in an elastic medium using Nonlocal Stress Gradient Theory [15]. Akgöz and Civelek studied the longitudinal free vibration problem of micro-bar using the Strain Gradient Elasticity Theory. They obtained the equation of motion and boundary conditions with Hamilton Principle [16]. Karlicic et al. analyzed free flexural vibration and buckling of SWCNTs under the effect of compressive axial loading. They used Reddy and Huu-Thai reformulated beam theories in equation of motions according to different gradient elasticity approaches like stress, strain and combined strain/inertia [17].

In this study, governing equations for torsional vibration will be obtained using stress, strain and combined gradient theories. Effect of the nonlocal parameters on vibration will be investigated and depicted in figures.

Analysis

1. Eringen's Nonlocal Theory

Eringen proposed the Nonlocal Elasticity Theory for including size effect and long range interactions [2, 3] in continuum. In order to account size dependence, the stress tensor in the nonlocal approach can be defined as [2]:

$$\tau_{ij}(x) = \int_V \chi(|x - x'|, \gamma) C_{ijkl} \varepsilon_{kl} dV(x'), \quad \forall x \in V, \tag{1}$$

where τ_{ij} is the nonlocal stress tensor, ε_{kl} is the strain tensor, C_{ijkl} elastic modulus tensor, $\chi(|x - x'|, \gamma)$ is the attenuation function and $|x - x'|$ is the Euclidean distance. $\mu = e_0 a$, where μ is nonlocal parameter, a is an internal characteristic length for CNT and e_0 is a constant. e_0 parameter can be adjusted using the dispersion curves based on the atomic models. For a specific material, geometry or problem the nonlocal parameter can be estimated by fitting the results of Atomic Lattice Dynamics [2, 18] and Molecular Dynamics [5, 19]. An estimation of the small scale parameter for a SWCNT was proposed in literature ($e_0a \leq 2$nm) [20].

One dimensional form of nonlocal stress and strain gradient relation in circumferential direction can be obtained in the light of Nonlocal Theory, as below:

$$\left(1-\mu_\tau \frac{\partial^2}{\partial x^2}\right)\tau = G\left(1+\mu_\gamma \frac{\partial^2}{\partial x^2}\right)\gamma \quad (2)$$

where γ is the local shear strain and τ is the local shear stress of CNT and μ_τ and μ_γ are the nonlocal stress and strain gradient parameter, respectively.

2. Equation of Motion

A nanotube with length (L) and diameter (d) is considered. The equation of motion in the circumferential direction can be written as [15]:

$$GI_P \frac{\partial^2\theta}{\partial x^2} = \rho I_P \frac{\partial^2\theta}{\partial t^2} \quad (3)$$

where G is the shear modulus, ρ is the density, I_P is the polar moment of inertia, θ is the angular displacement of CNT. The I_p is defined as:

$$I_P = \pi \frac{({R_2}^4 - {R_1}^4)}{2} \quad (4)$$

where R_1 and R_2 are the inner and outer radius of CNT respectively. If Eq. (3) is rearranged according to Eq. (2), one obtains:

$$GI_P\left(1+\mu_\gamma \frac{\partial^2}{\partial x^2}\right)\frac{\partial^2\theta}{\partial x^2} = \rho I_P \frac{\partial^2\theta}{\partial t^2}\left(1-\mu_\tau \frac{\partial^2}{\partial x^2}\right) \quad (5)$$

If Eq. (5) is rearranged, governing equation of motion for the torsional deformation according to both strain and inertia gradient theories is obtained. If the nonlocal stress gradient parameter is accepted as equal to zero ($\mu_\tau = 0$), the nonlocal strain gradient elasticity equation is obtained. If the nonlocal strain gradient parameter is accepted as equal to zero ($\mu_\gamma = 0$), the nonlocal stress gradient elasticity equation is obtained. If both nonlocal parameter is accepted as equal to zero ($\mu_\tau = \mu_\gamma = 0$), classical elasticity equation is obtained.

$$\mu_\gamma GI_P \frac{\partial^4\theta}{\partial x^4} + GI_P \frac{\partial^2\theta}{\partial x^2} + \mu_\tau \rho I_P \frac{\partial^4\theta}{\partial x^2 \partial t^2} - \rho I_P \frac{\partial^2\theta}{\partial t^2} = 0 \quad (6)$$

With the harmonic vibration assumption in the circumferential direction, displacement for each tube can be written as $\left(\bar{x} = \frac{x}{L}\right)$:

$$\theta_i(\bar{x},t) = A(\bar{x})_i\, e^{j\omega t} \quad (7)$$

where $A(\bar{x})$ is the angular displacement function, ω is the torsional frequency and $j^2=-1$. If Eq. (7) is rearranged according to Eq. (8) and non-dimensional parameters, one obtains:

$$\frac{\partial^4\theta}{\partial \bar{x}^4}\left[\frac{\mu_\gamma}{L^2}\right] + \frac{\partial^2\theta}{\partial \bar{x}^2}\left[1-\frac{\mu_\tau}{L^2}\Omega^2\right] + \theta[\Omega^2] = 0 \quad (8)$$

where Ω is the non-dimensional frequency parameter (NDFP) and defines as:

$$\Omega^2 = \frac{\rho\omega^2 L^2}{G} \quad (9)$$

For the Clamped-Clamped (C-C) boundary condition, the displacement function ($A(\bar{x})$) can be assumed as:

$$A(\bar{x}) = C\sin(n\pi\bar{x}) \quad (10)$$

where C is the amplitude of the displacement and n is the half wave number of vibration. If Eq. (8) rearranged according to Eq. (10), one obtains:

$$\left[(n\pi)^4\left(\frac{\mu_\gamma}{L^2}\right) - (n\pi)^2\left(1 - \frac{\mu_\tau}{L^2}\Omega^2\right) + (\Omega^2)\right] = 0 \quad (11)$$

Characteristic equation in Eq. (11) must be zero and non-dimensional frequency parameter which satisfy this condition, can be found with solving this equation.

3. Numerical Results and Discussion

In this section, validation of the present model is shown firstly. After that, variation of NDFP with nonlocal parameters is investigated. Effect of the nanotube length to the nonlocal behavior is also shown in figures.

Material properties of CNTs are selected as in the Table-1. There have been many researches about physical properties of CNTs. Shear Modulus for CNTs are selected from the Ref. [21]. Density(ρ) of CNTs is determined using the calculation method in Ref. [22]. CNT thickness is accepted as 0.066 nm according to Ref. [23].

Table 1
Material Properties for CNT

CNT	Inner Radius (nm)	Density (ρ) (kg/m^3)	Shear Modulus (G) (GPa)
Armchair (10x10)	0.68	10989	0.45

The torsional wave frequency results are compared with the Lattice Dynamics for the validation. Comparison can be seen in Fig. (1). Nonlocal combined gradient theory shows much better approximation when compared to the nonlocal stress and strain gradient theories and obviously local (classical) theory. Torsional vibration wave frequencies are obtained using Eqs. (12) and (13) [24] .

$$\omega_{LD} = \frac{2c}{a}\sqrt{sin^2\left(\frac{ka}{2}\right)} \quad (12)$$

$$\omega_{NL} = c\sqrt{\frac{k^2(1-\mu_\gamma k^2)}{1+\mu_\tau k^2}} \quad (13)$$

Eringen determined the e_0 parameter in stress gradient approach according to Lattice Dynamics results ($e_{0\tau}$=0.39). Same parameters for the strain gradient approach ($e_{0\varepsilon}$=0.25) and combined gradient approach ($e_{0\tau}$=0.20, $e_{0\varepsilon}$=0.21) can be determined using the Lattice Dynamics results.

MD Simulations results are obtained by Khademolhosseini's work [25]. Torsional frequencies are compared at different mode numbers (see Table-2). Present model gives very close results to MD simulation results.

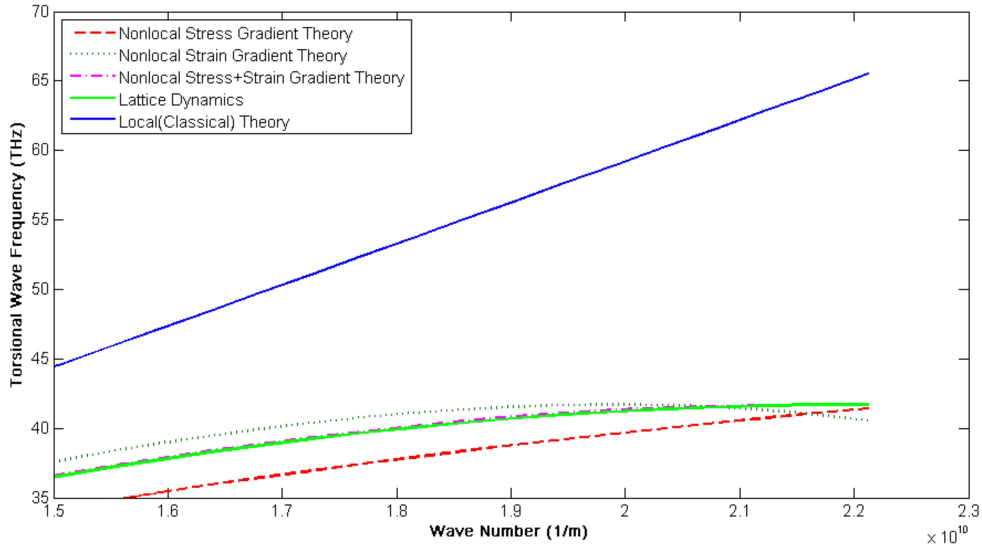

Fig. 1. Torsional Wave Propagation Dispersion Curves for Different Theories

Table 2
Comparison of Torsional Wave Frequencies (rad/s)

	Ref. [25]	Present Study		
Mode	MD Simulation	Nonlocal Stress	Nonlocal Strain	Nonlocal Combined
1	2.41×10^{12}	2.4340×10^{12}	2.4340×10^{12}	2.4340×10^{12}
4	9.62×10^{12}	9.7286×10^{12}	9.7331×10^{12}	9.7320×10^{12}

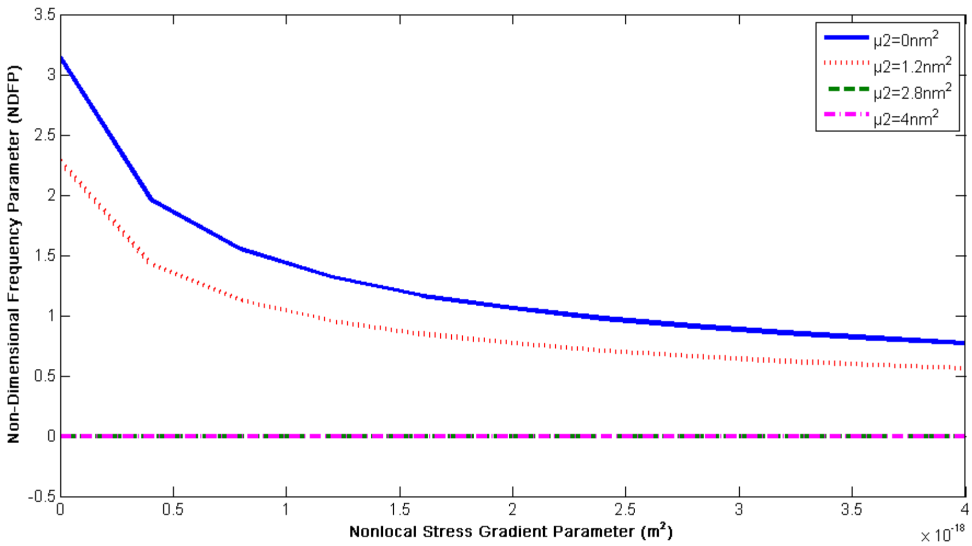

Fig. 2. Variation of NDFP with Nonlocal Stress and Strain Gradient Parameters (L=5nm)

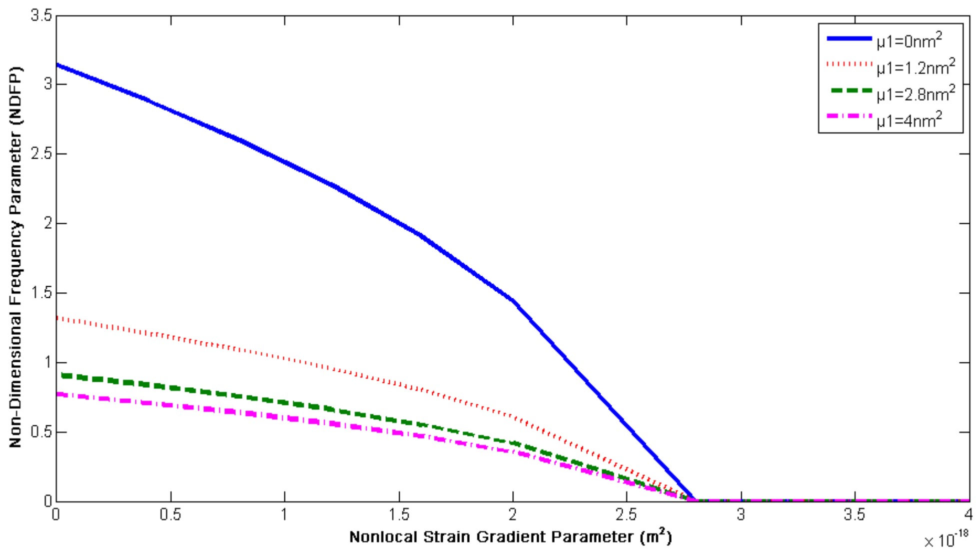

Fig. 3. Variation of NDFP with Nonlocal Stress and Strain Gradient Parameters (L=5nm)

Effect of the nonlocal stress and strain gradient parameters can be seen at Figs. (2-5). Both gradient theories decrease the NDFP with increasing nonlocal parameter. But in the stress gradient approach, NDFP value approaches a limit value for higher values of μ_τ ($\mu_\tau \gg 4nm^2$) contrary to strain gradient approach. CNT became stronger for strain gradient approach rather than the stress gradient. Especially in shorter nanotubes, NDFP approaches to zero with the effect of strain gradient nonlocal parameter. Also limit value for the NDFP in strain gradient approach must be zero at longer nanotube lengths ($\mu_\gamma \gg 4nm^2$).

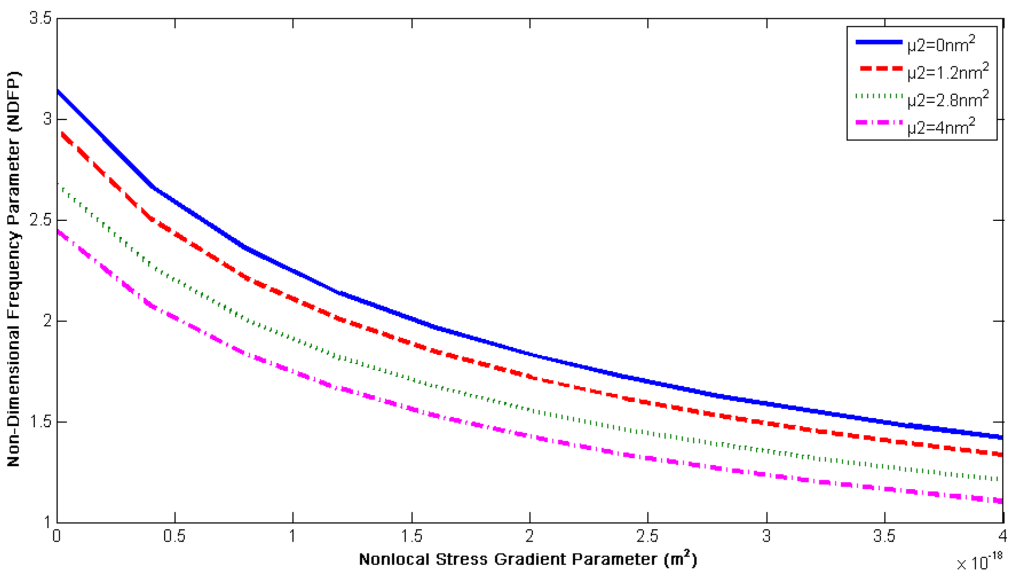

Fig. 4. Variation of NDFP with Nonlocal Stress and Strain Gradient Parameters (L=10nm)

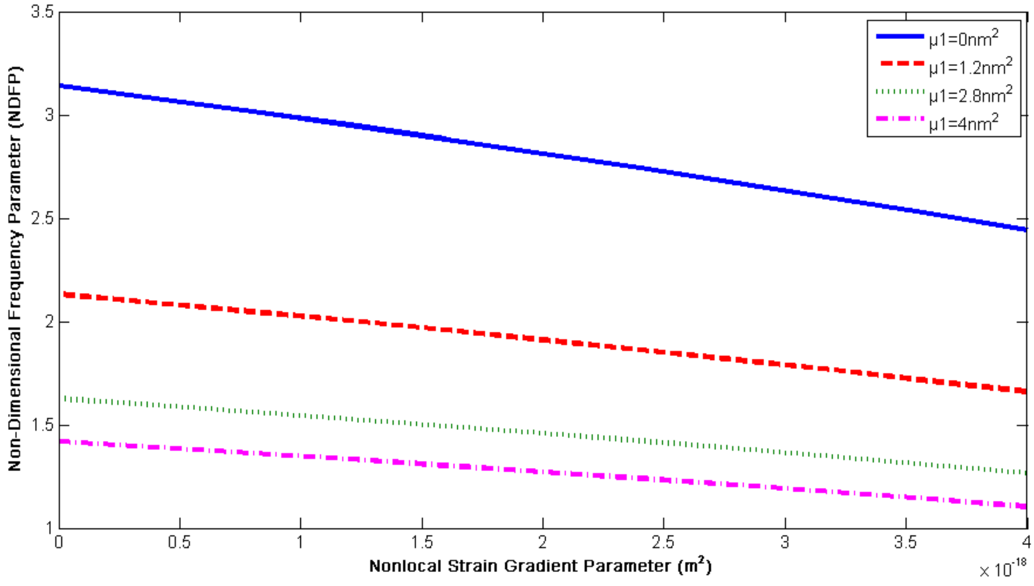

Fig. 5. Variation of NDFP with Nonlocal Stress and Strain Gradient Parameters (L=10nm)

In Figs. 6 and 7, nanotube length effect can be seen. Both nonlocal gradient theories are effective in shorter nanotube length. The nonlocal effect vanishes with increasing nanotube length and nonlocal results approaches to the local results, especially for bigger nanotube length values from 20nm.

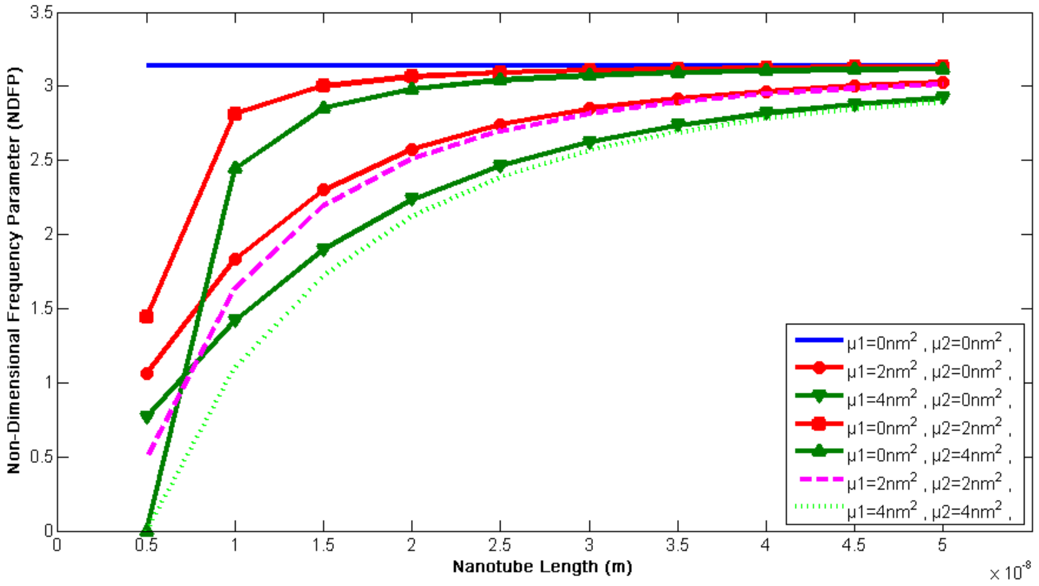

Fig. 6. Variation of NDFP with Nanotube Length

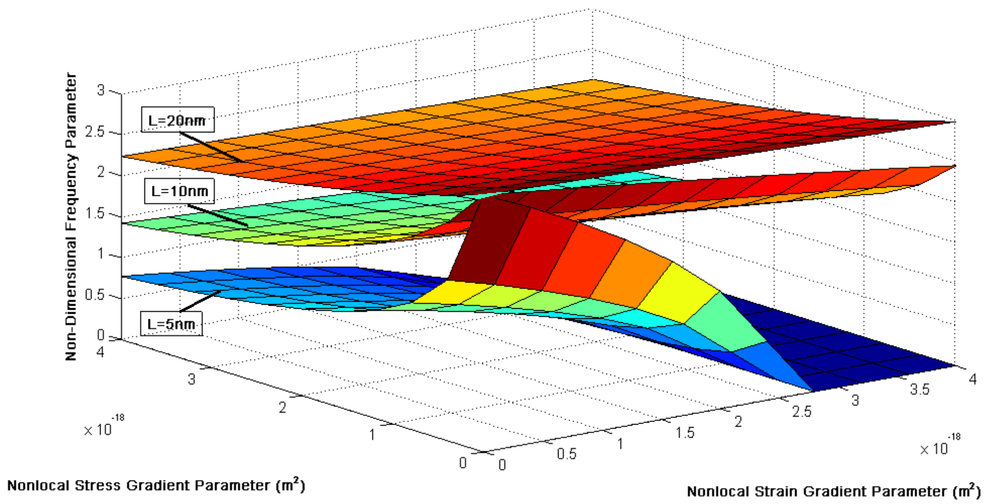

Fig. 7. Variation of NDFP with Nonlocal Stress and Strain Gradient Parameters

Conclusion

In the present study, torsional vibration of CNTs is investigated by using nonlocal stress gradient, nonlocal strain gradient and nonlocal combined (strain/inertia) gradient theories. Nonlocal effect decreases the NDFP in all cases. CNT is become stiffer with the effect of strain gradient theory. Nonlocal effect is more pronounced for CNTs for L<20nm. Combined nonlocal gradient theory shows much more agreement with Lattice Dynamics rather than the stress and strain gradient nonlocal theories. Present results can be useful for mechanical modeling of CNTs.

References

1. Iijima S. (1991) «Helical microtubules of graphitic carbon», Nature, Vol. 354, pp. 56–58. DOI: 10.1038/354056a0
2. Eringen A.C. (1983) «On differential equations of nonlocal elasticity and solutions of screw dislocation and surface waves», Journal of Applied Physics, Vol. 54, pp. 4703–4710. DOI: 10.1063/1.332803
3. Eringen A.C. (1972) «Nonlocal polar elastic continua», International Journal of Engineering Science, Vol. 10, pp. 1–16. DOI: 10.1016/0020-7225(72)90070-5
4. Wang Q., Varadan V.K. (2006) «Vibration of carbon nanotubes studied using nonlocal continuum mechanics», Smart Materials and Structures, Vol. 15, pp. 659–666. DOI: 10.1088/0964-1726/15/2/050
5. Duan W.H., Wang C.M., Zhang Y.Y. (2007) «Calibration of nonlocal scaling effect parameter for free vibration of carbon nanotubes by molecular dynamics», Journal of Applied Physics, Vol. 101, pp. 24305. DOI: 10.1063/1.2423140
6. Kumar D., Heinrich C., Waas A.M. (2008) «Buckling analysis of carbon nanotubes modeled using nonlocal continuum theories», Journal of Applied Physics, Vol. 103, pp. 1–9. DOI: 10.1063/1.2901201
7. Lim C.W. (2010) «On the truth of nanoscale for nanobeams based on nonlocal elastic stress field theory: Equilibrium, governing equation and static deflection», Applied Mathematics and Mechanics (English Edition), Vol. 31, pp. 37–54. DOI: 10.1007/s10483-010-0105-7
8. Şimşek M. (2010) «Vibration analysis of a single-walled carbon nanotube under action of a moving harmonic load based on nonlocal elasticity theory», Physica E: Low-dimensional Systems and Nanostructures, Vol. 43, pp. 182–191. DOI: 10.1016/j.physe.2010.07.003
9. Zhang Y.Y., Wang C.M., Challamel N. (2010) «Bending, Buckling, and Vibration

of Micro/Nanobeams by Hybrid Nonlocal Beam Model», Journal of Engineering Mechanics, Vol. 136, pp. 562–574. DOI: 10.1061/(ASCE)EM.1943-7889.0000107

10. Ansari R., Gholami R., Rouhi H. (2012) «Vibration analysis of single-walled carbon nanotubes using different gradient elasticity theories», Composites Part B: Engineering, Vol. 43, pp. 2985–2989. DOI: 10.1016/j.compositesb.2012.05.049

11. Thai H.T. (2012) «A nonlocal beam theory for bending, buckling, and vibration of nanobeams», International Journal of Engineering Science, Vol. 52, pp. 56–64. DOI: 10.1016/j.ijengsci.2011.11.011

12. Narendar S., Ravinder S., Gopalakrishnan S. (2012) «Strain gradient torsional vibration analysis of micro/nano rods», International Journal of Nano Dimension, Vol. 3, pp. 1–17. DOI: 10.7508/ijnd.2012.01.001

13. Wang L. (2012) «Vibration analysis of nanotubes conveying fluid based on gradient elasticity theory», Journal of Vibration and Control, Vol. 18, pp. 313–320. DOI: 10.1177/1077546311403957

14. Wang B.L., Wang K.F. (2013) «Vibration analysis of embedded nanotubes using nonlocal continuum theory», Composites Part B: Engineering, Vol. 47, pp. 96–101. DOI: 10.1016/j.compositesb.2012.10.043

15. Arda M., Aydogdu M. (2014) «Torsional statics and dynamics of nanotubes embedded in an elastic medium», Composite Structures, Vol. 114, pp. 80–91. DOI: 10.1016/j.compstruct.2014.03.053

16. Akgöz B., Civalek Ö. (2014) «Longitudinal vibration analysis for microbars based on strain gradient elasticity theory», Journal of Vibration and Control, Vol. 20, pp. 606–616. DOI: 10.1177/1077546312463752

17. Karličić D., Kozić P., Pavlović R. (2015) «Flexural vibration and buckling analysis of single-walled carbon nanotubes using different gradient elasticity theories based on Reddy and Huu-Tai formulations», Journal of Theoretical and Applied Mechanics, pp. 217. DOI: 10.15632/jtam-pl.53.1.217

18. Aydogdu M. (2012) «Longitudinal wave propagation in nanorods using a general nonlocal unimodal rod theory and calibration of nonlocal parameter with lattice dynamics», International Journal of Engineering Science, Vol. 56, pp. 17–28. DOI: 10.1016/j.ijengsci.2012.02.004

19. Wang L., Hu H. (2005) «Flexural wave propagation in single-walled carbon nanotubes», Phys Rev B, Vol. 71, pp. 195412. DOI: 10.1103/PhysRevB.71.195412

20. Wang Q., Wang C.M. (2007) «The constitutive relation and small scale parameter of nonlocal continuum mechanics for modelling carbon nanotubes», Nanotechnology, Vol. 18, pp. 75702. DOI: 10.1088/0957-4484/18/7/075702

21. Li C., Chou T.-W. (2003) «A structural mechanics approach for the analysis of carbon nanotubes», International Journal of Solids and Structures, Vol. 40, pp. 2487–2499. DOI: 10.1016/S0020-7683(03)00056-8

22. Laurent C., Flahaut E., Peigney a. (2010) «The weight and density of carbon nanotubes versus the number of walls and diameter», Carbon, Vol. 48, pp. 2994–2996. DOI: 10.1016/j.carbon.2010.04.010

23. Wang C.Y., Zhang L.C. (2008) «A critical assessment of the elastic properties and effective wall thickness of single-walled carbon nanotubes.», Nanotechnology, Vol. 19, pp. 75705. DOI: 10.1088/0957-4484/19/7/075705

24. Arda M., Aydogdu M. (2016) «Torsional wave propagation of CNTs via different nonlocal gradient theories», ICSV 2016 - 23rd Int. Congr. Sound Vib. From Anc. to Mod. Acoust.

25. Khademolhosseini F., Phani A.S., Nojeh A., Rajapakse N. (2012) «Nonlocal continuum modeling and molecular dynamics simulation of torsional vibration of carbon nanotubes», IEEE Transactions on Nanotechnology, Vol. 11, pp. 34–43. DOI: 10.1109/TNANO.2011.2111380