Computational continuum modelling to analysis the dynamic and static stability of a cantilever nano-scale system

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Abstract. Calculating size-dependent mechanical properties of the nano-scale materials usually involves cumbersome numerical and theoretical works. In this paper, we aim to present a closed-form relation to calculate the length-dependent Young's modulus of carbon nanotubes (CNTs) based on nonlocal elasticity theory. In this regard, a single wall carbon nanotube (SWCNT) is considered as a rod structure and the governing nonlocal equations are developed under uniaxial tensile load. The equations are solved using analytical methods and strain distribution, total displacement and the size-dependent equivalent Young's modulus are obtained. Further, the results are compared with the molecular dynamics results from the literature. The outcome indicates that the calculated relations are coincident with the molecular dynamics results.

Keywords: carbon nanotube; nanocomposite; nonlocal elasticity; size-dependent properties; stability; Young's modulus

1. Introduction

Carbon nanotubes have received considerable attention from researchers, and many reports have been published on their extraordinary mechanical, electrical and thermal properties (Habibi *et al.* 2016, 2018a, b, 2019b, d, e, Ebrahimi *et al.* 2019b, Esmailpoor Hajilak *et al.* 2019, Pourjabari *et al.* 2019, Safarpour *et al.* 2019a, Zhu *et al.* 2022, Zheng *et al.* 2023). The mechanical behavior of the carbon nanotubes have been analyzed through several methods including molecular dynamics and continuum mechanics, and these studies predicts noteworthy mechanical properties for these small materials (Fazaeli *et al.* 2016, Habibi *et al.* 2017, 2019a, c, Safarpour *et al.* 2018, 2019b, 2020, Alipour *et al.* 2020, Ebrahimi *et al.* 2020a, Ghazanfari *et al.* 2020, Chen *et al.* 2022). Owing to these mechanical properties, carbon nanotubes have the potential to be employed in many future devices and nanostructured materials. As an example, high Young modulus accompanied by their low density, makes them a good choice for reinforcing material in composites (Ebrahimi *et al.* 2019c, d, 2020b, Hashemi *et al.* 2019, Moayedi *et al.* 2019, 2020a, b, Mohammadgholiha *et al.* 2019, Mohammadi *et al.* 2019, Habibi *et al.* 2020, Oyarhossein *et al.* 2020, Shariati *et al.* 2020a, b, Shokrgozar *et al.* 2020).

Experimental studies as well as atomic simulations demonstrate that the mechanical properties

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of materials in nano scales are highly dependent on the sizes of these materials (Hashemi et al. 2019, Al-Furjan et al. 2020c, d, e, f, Bai et al. 2020, Cheshmeh et al. 2020, Li et al. 2020a, Lori et al. 2020, Najaafi et al. 2020, Shariati et al. 2020c, Xiong et al. 2020, Guo et al. 2021b, Liu et al. 2021a). Carbon nanotubes, as nanoscale materials, also have size dependent properties (Adamian et al. 2020, Al-Furjan et al. 2020a, b, Li et al. 2020b, Liu et al. 2020b, 2021b, Zare et al. 2020, Dai et al. 2021b, Habibi et al. 2021, Heidari et al. 2021, Huang et al. 2021a, Zhang et al. 2021). Lee et al (2007) measured the elastic modulus of multi wall carbon nanotubes (MWCNTs) grown by catalytic chemical vapor deposition (CVD), and it is observed that 10-25 nm diameter MWCNTs exhibit considerable diameter dependent elastic modulus. They demonstrated that the elastic modulus of the MWCNTs decreases with increase in the diameter. On the other hand, atomic simulations show that the elastic modulus of 1-2nm diameter CNTs increases with increase in the diameter (Chang and Gao 2003). It is argued that the increase in elastic modulus in small diameter (<1.5 nm) is due to the excessive strain imposed on the graphene shells, and this effect is not prevalent in the experimental results that deal with 10-25 nm nanotubes. (Chang and Gao 2003) presented an analytical method based on molecular dynamics to calculate the elastic properties of carbon nanotubes as a function of their geometry parameters such as diameter and chirality. The results indicate that the Young modulus of SWCNT increases with increase in diameter and then converges to a constant value for large diameters. (Li and Chou 2003) calculated the young and shear modulus of single layer carbon nanotubes using a structural mechanics method. In their analysis, a C-C bond is modeled as a beam with specific Young, bending and shear moduli that were calculated by matching beam specifications with force field constants. Using this method, they observed that the Young modulus of CNTs reduces with increase in diameter. The shear modulus also shows similar dependency on the diameter. In recent years, length dependent properties of SWCNT is investigated by (Naumov et al. 2013, Rao et al. 2015, Zhu and Li 2017, Taati et al. 2020) and (Ranjbartoreh and Wang 2010). Anandatheertha et al. (2010) used molecular dynamics based finite element method to evaluate Young modulus of SWCNT. In lengths smaller than 60 nm, the Young modulus exhibits an increase when increasing in length of the CNT, and for longer lengths, it converges to a constant value. (Ranjbartoreh and Wang 2010) employed molecular dynamics simulation to predict behavior of SWCNT under various loading conditions. The results show that the Young modulus increases with increase in the length. There can be found several research works on the size dependent vibrational and buckling behavior of CNTs and CNT-reinforced nano-composites employing nonlocal and gradient theories of elasticity (Hosseini et al. 2017, 2018, Aydogdu et al. 2018, Boutaleb et al. 2019, Ebrahimi et al. 2019a, Soni et al. 2020). Nonlocal theory is also employed in obtaining size-dependent responses of properties other than mechanical ones. Coupled magnetic, thermal and elasticity responses in shape memory alloyed was investigated by Lata and Singh (2021, 2022)

In investigating the mechanical properties of CNTs, the classical continuum based modeling has also been adopted by many researchers (Liu *et al.* 2020a, Wang *et al.* 2020, Zhou *et al.* 2020, Dai *et al.* 2021a, Guo *et al.* 2021a, Shao *et al.* 2021, Wu and Habibi 2021, Kong *et al.* 2022). Employing classical theory of elasticity instead of atomic simulation, some complicated mechanical behavior such as vibrations and buckling of CNTs can be studied (Shariati *et al.* 2012, 2016a, b, Shariati *et al.* 2019, 2020d, e, f, g, h, i, j, 2021a, b, Fan *et al.* 2022, Luo *et al.* 2022b, Wang *et al.* 2022a, Xia *et al.* 2022). Another virtue of employing the classical theory of elasticity is that it has less computational costs than the atomic simulations. However, the classical continuum modeling cannot reflect the size dependency of properties in nano materials. In the constitutive equation of the classical continuum theory, the stress is assumed a function of the local

strain, so nonlocal effects and size parameters are not observed in the equations of the classical elasticity theory. Nonlocal theory of elasticity (Eringen 1972) incorporating an internal length scale parameter into the constitutive equation, presents size-dependent mechanical properties in nano materials (Chaht et al. 2015, Zenkour and Abouelregal 2015, Lata and Singh 2019, Pham et al. 2021). Pisano and Fuschi (2003) presented a nonlocal formulation for a bar under uniaxial tension and their results indicated a non-uniform strain distribution in the bar. Failla et al. (2010) used approximate methods in order to obtain strain, displacement and strain energy in a nonlocal bar under uniaxial tension. After (Peddieson et al. 2003), the size dependent nonlocal theory of elasticity has been widely used in predicting mechanical behavior of nanomaterials. They formulated the deflection equation of a nonlocal Bernoulli-Euler beam, and showed that based on the nonlocal elasticity theory, the nonlocal effect manifest itself in the nano-scale devices. Sudak (2003) investigated the buckling of a multiwall carbon nanotube (MWCNT) using nonlocal elasticity theory. In the analysis, each individual CNT is modeled as a column and the buckling of the MWCNT is investigated by considering the interaction between adjacent CNTs as van der Walls interaction. The results demonstrated that the critical load of buckling is highly dependent on the scale parameter. In these studies, the results of the nonlocal elasticity are more conservative than those of the classical elasticity. Wang et al. (2006) investigated buckling of CNTs using both nonlocal column and shell models. In the nonlocal shell model, the critical load is found to be function of diameter as well as length of the CNT, where the column model cannot reflect the dependency of critical load on the diameter. Zhang et al. (2005) investigated free vibrations of DWCNT using nonlocal elasticity theory. Each CNT was modeled as a nonlocal beam and the interaction between two CNT is modeled as spring with a specific coefficient. They concluded that the classical theory of elasticity could overestimate the amount of the natural frequencies.

In nanocomposite materials, which are frequently reinforced with CNTs and other nanostructures, elasticity parameters are usually considered as constants (Bellal *et al.* 2020, Matouk *et al.* 2020, Rouabhia *et al.* 2020, Bouafia *et al.* 2021, Heidari *et al.* 2021, Kumar *et al.* 2021, Van Vinh and Tounsi 2021, Bendaida *et al.* 2022). However, a size dependent properties are more desirable in this context. Using embedded size-dependent theories in analyzing nanocomposite puts extra computational costs in calculation which could be easily avoided using approximate or exact closed-form relations (Al-Furjan *et al.* 2021). On the other hand, in chemical production of nanostructures, it is barely possible to control size of each nanostructure (Al-Furjan *et al.* 2020, Bourada *et al.* 2022, Bousahla Abdelmoumen *et al.* 2020, Asgharnejad Lamraski *et al.* 2022, Moradi *et al.* 2022a, b, Vatanpour *et al.* 2022a, b). Moreover, novel methods of evaluating size and effects of nanostructures and nanoparticles are commonly relies on statistical approximations (Lingamdinne *et al.* 2023). Using numerical methods like finite element has its own drawbacks in terms of computational, accuracy and modeling time (Amelirad and Assempour 2019, 2021).

In this paper, the dependency of Young modulus of elasticity of CNTs on length is investigated via nonlocal elasticity theory. The exact size dependency of CNTs are often calculated from molecular dynamics simulation. However, in practical problems, like composite structures, a closed form relation is required to reduce computational costs. Specifically, in mass production of CNTs, length control of CNTs are very complicated. The closed form relation could be used in statistical analyses as well as simulating a portion of nanocomposites with limited number of CNTs. In this way, the nonlocal bar model is employed and a uniaxial tension is applied to two ends of the bar. A specific version of nonlocal constitutive equation is employed in order to

calculate the nonuniform strain distribution along the length of the CNT. The governing equation of the nonlocal bar turns out to be a Volttera integral equation that is solved using analytical methods. Finally, The Young modulus of CNT is calculated by dividing the applied stress by the average amount of strain in the bar. The effects of the nonlocal parameters are studied and results are compared with the results of molecular dynamics based finite elements method.

2. Nonlocal theory of elasticity

Nonlocal theory of elasticity is one the theories that take into account the effects of the size in the mechanical properties (Ma *et al.* 2022, Zhao *et al.* 2022, Hou *et al.* 2021, Huang *et al.* 2021b, c, Jiao *et al.* 2021, Liu *et al.* 2021c, Moradi *et al.* 2021, Xu *et al.* 2021, Dong *et al.* 2022, Fan *et al.* 2022, Luo *et al.* 2022a, Luo *et al.* 2022b, Michael *et al.* 2022, Wang *et al.* 2022b, c, Yang *et al.* 2022a, b, Yu *et al.* 2022, Zheng *et al.* 2022, Zhu *et al.* 2022). The essence of incorporating size effects in the mechanical properties is that the stress at a point of the material is considered to be affected by not only the local strain but also the nonlocal strain field. The influence of the nonlocal strain is imposed on the stress by employing an attenuation function. In this way, strain at farther points (compared to internal characteristic length) has less influence on the stress than strain at the points near the reference point. The constitutive equation of a nonlocal linear homogenous elastic solid is given as follows:

$$\sigma_{ij}(\mathbf{x}) = \int_{\Omega} \alpha(|\mathbf{x} - \mathbf{x}'|) C_{ijkl} \varepsilon_{kl}(\mathbf{x}') \, d\Omega(\mathbf{x}') \tag{1}$$

where σ_{ij} are the nonlocal stress components, and ε_{ij} are the strain components for infinitesimal displacement components, and they are defined by the following equation:

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} \right) \tag{2}$$

where u_i are the displacement vector components. The fourth order tensor C_{ijkl} is the elasticity tensor of the classical elasticity (Fan *et al.* 2022, Luo *et al.* 2022b, Wang *et al.* 2022a, Xia *et al.* 2022).

As mentioned above, the influence of the nonlocal strain on the stress at point x is incorporated by an attenuation function $\alpha(|x - x'|)$. The attenuation function $\alpha(|x - x'|)$ is a positive scalar function of the Euclidean distance between point x' and the reference point x. When the Euclidean distance is very large compared to internal length $|x - x'| \rightarrow \infty$ the attenuation function vanishes $\alpha \rightarrow 0$. However, in practice, the influence of nonlocal strain after an specific distance, called influence distance, vanishes, so that the attenuation function after that distance become $\alpha(|x - x'|) \approx 0$ (Polizzotto 2001). For small distances, the value of the attenuation function α is considerable whereas at large distances the nonlocality effects substantially decrease. The influence distance is characterized by the internal characteristic length, and it is in the same order of the internal characteristic length. It is expected when the influence distance vanishes so that only local strain takes into account, the constitutive Eq. (1) become the local form of:

$$\sigma_{ij}(\mathbf{x}) = C_{ijkl} \varepsilon_{kl}(\mathbf{x}) \tag{3}$$

80

The attenuation function should fulfill the following condition:

$$\int_{\Omega_{\infty}} \alpha(|\boldsymbol{x} - \boldsymbol{x}'|) \, d\Omega = 1 \tag{4}$$

The domain Ω_{∞} is an infinite domain contain the Ω . There are some types of functions that can be employed for attenuation function (Eringen 2002):

$$\alpha(r) = A \exp\left(1 - \frac{r}{l}\right) \tag{5}$$

$$\alpha(r) = A\left(1 - \frac{r^2}{l^2}\right) \tag{6}$$

$$\alpha(r) = A\left(1 - \frac{r}{l}\right) \tag{7}$$

where the constant l is related to the internal characteristic length and the constant Acan be calculated using Eq. (4). In this article, the following form of the attenuation function is used (Altan 1989):

$$\alpha(r) = \zeta_1 \delta(r) + \zeta_2 \bar{\alpha}(r) \tag{8}$$

that gives the following constitutive equation:

$$\sigma_{ij}(\mathbf{x}) = \zeta_1 C_{ijkl} \varepsilon_{kl}(\mathbf{x}) + \zeta_2 \int_{\Omega} \overline{\alpha}(|\mathbf{x} - \mathbf{x}'|) C_{ijkl} \varepsilon_{kl}(\mathbf{x}') d\Omega(\mathbf{x}')$$
⁽⁹⁾

Two constants ζ_1 and ζ_2 are the positive material constants with the constraint $\zeta_1 + \zeta_2 = 1$. Indeed, using influence function of Eq. (8), the material is conceived to be a two phase material. The first phase with influence factor ζ_1 represents the local part of influence function and consequently, the local part of constitutive Eq. (9). The second phase with influence factor ζ_2 represents the nonlocal part of influence function and constitutive Eq. (9). Applying condition of Eq. (4), it can be easily seen that the same condition should be imposed on $\bar{\alpha}$, that is:

$$\int_{\Omega_{\infty}} \bar{\alpha}(|\boldsymbol{x} - \boldsymbol{x}'|) \, d\Omega = 1 \tag{10}$$

3. Nonlocal elastic bar in tension

In this section, we consider an SWCNT with length L under uniaxial tension, as shown in Fig. 1a. For simplicity, the CNT is modeled as a one-dimensional nonlocal bar in tension under applied stress $\bar{\sigma}$ (Fig. 1b), and one end of it is pinned at (x = 0). From equilibrium of the bar, it is concluded that the internal stress of the CNT is uniform and equals the applied stress $\bar{\sigma}$. The one-dimensional form of Eqs. (9) and (2) is as Eqs. (11) and (12), respectively:

$$\sigma(x) = \zeta_1 E \varepsilon(x) + \zeta_2 \int_0^L \bar{\alpha}(|x - x'|) E \varepsilon(x') dx'$$
(11)

$$\varepsilon(x) = \frac{du}{dx} \tag{12}$$

where E is the Young modulus of the classical elasticity. For the one-dimensional bar in tension the stress $\sigma(x) = \overline{\sigma}$ and the strain in the bar is obtained from equation (11):

$$\varepsilon(x) = \frac{\bar{\sigma}}{\zeta_1 E} - \frac{\zeta_2}{\zeta_1} \int_0^L \bar{\alpha}(|x - x'|) \,\varepsilon(x') dx' \tag{13}$$

This equation is the Fredholm equation of the second kind and it is indicated that, despite the fact that the stress state in the CNT is uniform, the strain is not uniform in the CNT. A solution for this equation with following form for attenuation function $\bar{\alpha}$ is given by (Pisano and Fuschi 2003).

$$\bar{\alpha}(r) = A \exp\left(-\frac{r}{l}\right) \tag{14}$$

And, the solution for Eq. (13) is given by the following equation (Pisano and Fuschi 2003):

$$\varepsilon(x) = \frac{\bar{\sigma}}{E} \left\{ 1 + \frac{\zeta_2}{4\zeta_1} \left[e^{-\frac{x}{l} \left(\frac{\zeta_2}{2\zeta_1} + 1\right)} + e^{-\frac{L-x}{l} \left(\frac{\zeta_2}{2\zeta_1} + 1\right)} \right] \right\}$$
(15)

Using Eq. (15) and integrating Eq. (12) the displacement for each point is obtained:

$$u(x) = \frac{\bar{\sigma}L}{E} \begin{cases} \frac{x}{L} - \frac{l}{L} \frac{\frac{\zeta_2}{2\zeta_1}}{2(\frac{\zeta_2}{2\zeta_1} + 1)} \times \\ \left[e^{-\frac{x}{l}(\frac{\zeta_2}{2\zeta_1} + 1)} - e^{-\frac{L-x}{l}(\frac{\zeta_2}{2\zeta_1} + 1)} + e^{-\frac{L}{l}(\frac{\zeta_2}{2\zeta_1} + 1)} - 1 \right] \end{cases}$$
(16)

In order to calculate the Young modulus of the CNT, the applied stress is divided by the average strain inside the bar. The average strain of the CNT is obtained by following relation:

$$\varepsilon_{ave} = \frac{1}{L} \int_0^L \varepsilon(x) dx = \frac{u(L)}{L}$$

$$= \overline{\varepsilon} \left\{ 1 - \frac{l}{L} \frac{\zeta_2 / 2\zeta_1}{(\zeta_2 / 2\zeta_1 + 1)} \left[e^{-\frac{L}{l} \left(\frac{\zeta_2}{2\zeta_1} + 1\right)} - 1 \right] \right\}$$
(17)

where the $\bar{\varepsilon}$ is the strain field produced with considering the classical constitutive equation that is $\bar{\varepsilon} = \bar{\sigma}/E$. Finally, the Young modulus of the CNT can be obtained as follows:

$$\frac{E^{nl}}{E} = \left\{ 1 - \frac{l}{L} \frac{\frac{\zeta_2}{2\zeta_1}}{\left(\frac{\zeta_2}{2\zeta_1} + 1\right)} \left[e^{-\frac{L}{l} \left(\frac{\zeta_2}{2\zeta_1} + 1\right)} - 1 \right] \right\}^{-1}$$
(18)

where E^{nl} is the Young modulus of the CNT in the nonlocal elasticity theory. As seen, this equation gives the Young modulus of CNT as a function of the length of the CNT *L*. It can also be concluded that when L/l >> 1, the length of the CNT is larger than the characteristic length, the calculated Young modulus for nonlocal elasticity tends to become equal to the classical Young modulus.

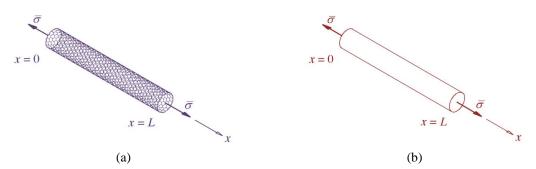


Fig. 1 (a) A CNT under uniaxial tension, (b) A bar model represented the CNT under uniaxial tension

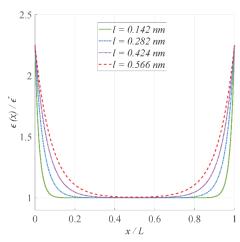


Fig. 2 Non-dimensional strain field in the CNT under uniaxial tension for L = 5nm, $\zeta_2/\zeta_1 = 5$, and various values of internal characteristic length l

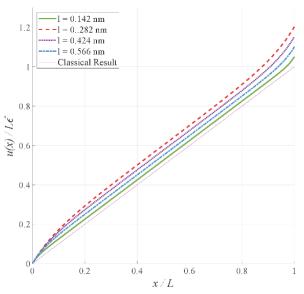


Fig. 3 Non-dimensional displacement along x-axis in the CNT under uniaxial tension for L = 5nm, $\zeta_2/\zeta_1 = 5$, and various values of internal characteristic length l

Jiangjiang Li

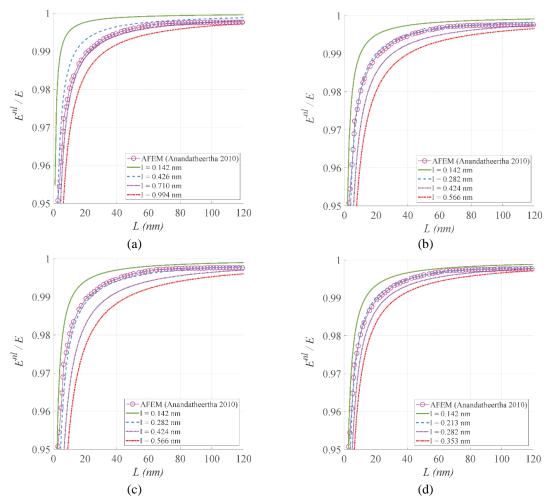


Fig. 4 Nondimensional Young modulus of the CNT under uniaxial tension as a function of length *L* for different values of internal characteristic length *l* and ζ_2/ζ_1 , (a) $\zeta_2/\zeta_1 = 1$, (b) $\zeta_2/\zeta_1 = 5$, (c) $\zeta_2/\zeta_1 = 10$, (d) $\zeta_2/\zeta_1 = 50$

4. Numerical results and discussion

In this section, the numerical results of the nonlocal theory of elasticity for length dependent Young modulus of the CNT are presented. Eqs. (15) and (16) give the strain and displacement fields in the CNT as functions of the x, respectively, and they are shown in Figs. 2 and 3. As seen, at regions near the boundaries the nonlocal results differ significantly from the classical values. These differences near the boundaries are due to "boundary effects" that is discussed in details by (Pisano and Fuschi 2003). Briefly, at the region near the boundaries, the boundaries cut the influence distance and influence regions out of boundaries have no effect on the state inside the bar. On the other hand, at the region far from boundaries the all points of the influence region located inside the medium. Consequently, the strain and displacement behaviors at the boundary region are different from inside the bar. As seen in Fig. 3, the displacement at x/L = 1 in nonlocal results is greater than classical one that is the nonlocal elasticity predicts softer behavior for CNTs under uniaxial tension.

Eq. (18) gives the Young's modulus of the CNT as a function of CNT length. In figure through figure, the dependency of the Young modulus of the CNT on the length is presented. The results show that the Young modulus of the CNT is highly dependent on the length and its value increases with increasing the length, and it converges to the amount of *E* independently from the length, internal characteristic length and ζ_2/ζ_1 . In these results, we omit to discuss on amount of the area of the CNT, and only the ratio of the Young modulus to its local value *E* is presented. The amount of *E* could be conceived as the Young modulus of a long CNT that was measured earlier (Yu *et al.* 2000).

As seen, the amount of non-dimensional Young's modulus of the CNT for length longer than 80 nm is independent of length. In fact, the results converges to the local elasticity theory which is indicates the applicability of the local theory of elasticity in large scales. On the over hand, in small lengths the results is highly dependent on the length, which demonstrate the role of nonlocality effects in the small scales. It should be mentioned that the internal characteristic length and the volume ratio are the material characteristics and their values are constant for a specific material. Because of lack of information on the exact values for these constants in CNTs, the different values presented here for internal characteristic length and ζ_2/ζ_1 in order to compare the current results with the result of the molecular dynamics based finite elements method (Anandatheertha *et al.* 2010). As seen in the figures, for some proper pair of the internal characteristic length and ζ_2/ζ_1 , the results of the nonlocal theory overlap with the result of the molecular dynamics based finite elements method.

5. Conclusions

Based on earlier experiments and simulations the mechanical properties of nanomaterials such as carbon nanotubes are strongly dependent on length scales. The classical elasticity theory, because of its intrinsic nature, cannot present a size dependent result. In this paper, using nonlocal theory of elasticity, dependency of Young elasticity modulus of CNT on the length was investigated. The size exact size dependent of CNTs are often calculated from molecular dynamics simulation. However, in practical problems, like composite structures, a closed form relation is required to reduce computational costs. In practical application of mass production of CNTs, length control of CNTs are very complicated. The closed form relation in this applications could be useful in statistical analyses as well as simulating a portion of nanocomposites with limited number of CNTs. The CNT was modeled as a nonlocal uniform bar in tension. The nonlocal theory of elasticity was presented and applied to formulate the one dimensional stress-strain relation inside the CNT. Using an analytical solution of the equation obtained for the strain filed in the CNT, a closed form relation was obtained for the Young modulus. The results show that the state of strain and displacement at the regions near boundaries of the bar in the nonlocal theory of elasticity are different significantly from classical ones so that these differences result in prediction of softer behavior for CNTs in the nonlocal theory. However, in the regions far from the boundaries, strain and displacement behaviors are similar to the classical ones. The amount of differences are dependent on the length of the CNT. From the stain field, it is determined that the Young modulus of CNTs are highly dependent on the length, and this dependency is such that by increasing the length of the CNT the Young modulus increased so that for the long lengths (greater

than 80 nm) the Young modulus, independent of length and nonlocal parameters, converges to a special amount. It can be concluded that from the nonlocal elasticity view point, the variation of Young modulus of CNTs are primarily due to the "boundary effects". The agreement of the nonlocal elasticity results with molecular dynamics based finite element method for, show that the nonlocal elasticity theory has a good potential in analyzing mechanical behavior of CNTs.

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86

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