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Computational analysis of molecular dynamics results in a fuzzy stability system

C.C. Hung[1], T. Nguyễn[2] and C.Y. Hsieh*[3]

[1]*Faculty of National Hsin Hua Senior High School, Tainan, Taiwan*
[2]*Ha Tinh University, Dai Nai Ward, Ha Tinh City, Vietnam*
[3]*National Pingtung University Education School, No.4-18, Minsheng Rd., Pingtung City, Pingtung County 900391, Taiwan*

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Abstract. 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. Therefore, we empathize and manually derive the results which shows the utilized lemma and criterion are believed effective and efficient for aircraft structural analysis of composite and nonlinear scenarios. To be fair, the experiment by numerical computation and calculations were explained the perfectness of the methodology we provided in the research.

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 (Zhao *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 (Alimoradzadeh *et al*. 2023, Jafari *et al*. 2023, Khosravikhor *et al*. 2023, Al-Jaafari *et al*. 2023, Shih 2012, 2023). 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 (Lee 2012, 2023, Lin 2009, 2013, Liu 2013, 2023, Akbari *et al*. 2023, Aksoylu *et al*. 2023).

Materials in nano scales are highly dependent on the sizes of these materials (Chandrasekaran *et al*. 2023, Chen *et al*. 2023a, b, Hsu 2013, Kuan 2012, Chen 2013, Cheng 2023). Carbon nanotubes, as nanoscale materials, also have size dependent properties (Chiou 2023, Fard *et al*. 2023, Gholizadeh *et al*. 2023, Ayough *et al*. 2023, Bai *et al*. 2023, Kuo 2010). Lee *et al* (2007) measured

*Corresponding author, Ph.D., E-mail: zykj_zywd@163.com

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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 (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 (Abad *et al*. 2023, Zou 2023, Banh *et al*. 2023, Behshad *et al*. 2023, Biao *et al*. 2023, Bounouara *et al*. 2023). 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 (Cánovas-González *et al*. 2023, Hong *et al*. 2023, Chen 2014, Chiang 2010, 2011, Zhang *et al*. 2023, Chen 2009). On the other hand, in chemical production of nanostructures, it is barely possible to control size of each nanostructure (Hsiao 2005, Tsai 2008, 2023, Yeh 2013, Zaoui *et al*. 2023, Zhan *et al*. 2023). Moreover, novel methods of evaluating size and effects of nanostructures and nanoparticles are commonly relies on statistical approximations (Ling *et al*. 2023). Using numerical methods like finite element has its own drawbacks in terms of computational, accuracy and modeling time (Amelirad 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 (Hsiao 2005, Tsai 2008, Tsai 2023, Yeh 2013, Zaoui *et al*. 2023, Zhan *et al*. 2023). 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:

$$\sigma_{ij}(\boldsymbol{x}) = \int \alpha(|\boldsymbol{x} - \boldsymbol{x}'|) C_{ijkl\ kl}(\boldsymbol{x}') d\Omega(\boldsymbol{x}') \tag{2.1}$$

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

$$ij = -\left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i}\right) \tag{2.2}$$

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 $\boldsymbol{x}$ is incorporated by an attenuation function $\alpha(|\boldsymbol{x} - \boldsymbol{x}'|)$. The attenuation function $\alpha(|\boldsymbol{x} - \boldsymbol{x}'|)$ is a positive scalar function of the Euclidean distance between point $\boldsymbol{x}'$ and the reference point $\boldsymbol{x}$. When the Euclidean distance is very large compared to internal length $|\boldsymbol{x} - \boldsymbol{x}'| \to \infty$ the attenuation function vanishes $\alpha \to 0$. 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 $\alpha(|\boldsymbol{x} - \boldsymbol{x}'|) \simeq 0$ (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:

$$\sigma ij(\boldsymbol{x}) = Cijkl\ kl(\boldsymbol{x}) \tag{2.3}$$

The attenuation function should fulfill the following condition:

$$\int \alpha(|\boldsymbol{x} - \boldsymbol{x}'|) d\Omega = 1 \tag{2.4}$$

3. Nonlocal fuzzy stability system

The fuzzy controller of the *j*th subsystem is in the following form:

Rule *i*: IF $x_{1j}(t)$ is M_{i1j} and $\cdots$ and $x_{gj}(t)$ is M_{igj}

$$\text{Then } u_j(t) = -K_{ij} x_j(t) \tag{3.1}$$

where $i = 1, 2, \cdots, r_j$. Hence, the final output of the fuzzy controller is

$$u_j(t) = -\frac{\sum_{i=1}^{r_j} w_{ij}(t) K_{ij} x_j(t)}{\sum_{i=1}^{r_j} w_{ij}(t)} = -\sum_{i=1}^{r_j} h_{ij}(t) K_{ij} x_j(t). \tag{3.2}$$

Substituting Eq. (3.2) into Eq. (2.4), we have the jth closed-loop subsystem:

$$\dot{x}_j(t) = \sum_{i=1}^{r_j} \sum_{f=1}^{r_j} h_{ij}(t) h_{fj}(t) [A_{ij} - B_{ij} K_{fj}] x_j(t) + \phi_j(t). \tag{3.3}$$

A stability criterion is given below to guarantee the asymptotic stability of the fuzzy large-scale system ***F***.

Theorem 1: The fuzzy large-scale system ***F*** is asymptotically stable, if the feedback gains (K_{ij}) are chosen to satisfy

$$\hat{\lambda}_{ij} = \lambda_m(Q_{ij}) - \beta_j > 0 \quad \text{and} \quad \tilde{\lambda}_{ifj} = \lambda_m(Q_{ifj}) - \beta_j > 0$$
$$\text{for } i = 1, 2, \cdots, r_j;\ i < f \le r_j;\ j = 1, 2, \cdots, J \tag{3.4}$$

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.

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 based on Li (2023), for which, 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. Moreover, the coupled in and out states matrices among three aviation stability are

$$C_{21} = \begin{bmatrix} 1.5 & -2.1 \\ -1 & 3 \end{bmatrix},\ C_{31} = \begin{bmatrix} 5 & 4.5 \\ 3 & 2.5 \end{bmatrix},\ C_{12} = \begin{bmatrix} 2 & -3 \\ -1.4 & 1.5 \end{bmatrix},$$
$$C_{32} = \begin{bmatrix} 1 & -2.4 \\ -1.4 & 1.2 \end{bmatrix},\ C_{13} = \begin{bmatrix} 2 & -0.5 \\ -0.6 & 0.5 \end{bmatrix},\ C_{23} = \begin{bmatrix} 1 & -1.4 \\ 1.2 & -0.3 \end{bmatrix}.$$

Therefore, aviation stability from coupled systems have the states matrices A_{ij} and B_{ij}.

Since the pairs (A_{ij}, B_{ij}), $i = 1, 2$; $j = 1, 2, 3$ are all given, we analyze controlled coupled structures as

Rule 1: If $x_{11}(t)$ is M_{111} Then $u_1(t) = -K_{11} x_1(t)$,

Rule 2: If $x_{11}(t)$ is M_{211} Then $u_1(t) = -K_{21} x_1(t)$.

$K_{11} = [-11.4815 \quad -0.3704]$ and $K_{21} = [-0.5161 \quad 0.1548]$.

Rule 1: If $x_{12}(t)$ is M_{112} Then $u_2(t) = -K_{12}x_2(t)$,

Rule 2: If $x_{12}(t)$ is M_{212} Then $u_2(t) = -K_{22}x_2(t)$,

$K_{12} = [-14.2857 \quad -0.5714]$ and $K_{22} = [0.5495 \quad -1.5568]$.

Rule 1: If $x_{13}(t)$ is M_{113} Then $u_3(t) = -K_{13}x_3(t)$,

Rule 2: If $x_{13}(t)$ is M_{213} Then $u_3(t) = -K_{23}x_3(t)$.

$K_{13} = [-4.0426 \quad -3.6170]$ and $K_{23} = [-11.7542 \quad -1.4213]$.

In order to satisfy the aviation stability conditions from coupled system of Theorem 1, Eq. must be positive we can obtain Q_{ij}, $i = 1, 2$; $j = 1, 2, 3$ positive definite:

$$P_1 = \begin{bmatrix} 1.5062 & -0.2794 \\ -0.2794 & 1.7619 \end{bmatrix},\ P_2 = \begin{bmatrix} 1.3865 & 0.3153 \\ 0.3153 & 1.4738 \end{bmatrix},\ P_3 = \begin{bmatrix} 1.3662 & 0.0876 \\ 0.0876 & 1.9350 \end{bmatrix}.$$

$$Q_{11} = \begin{bmatrix} 58.9131 & 23.3305 \\ 23.3305 & 45.5584 \end{bmatrix},\ Q_{21} = \begin{bmatrix} 77.9267 & -14.5195 \\ -14.5195 & 47.6183 \end{bmatrix},\ Q_{121} = \begin{bmatrix} 80.9133 & -24.5816 \\ -24.5816 & 43.7829 \end{bmatrix},$$

$$Q_{12} = \begin{bmatrix} 60.4030 & -23.0437 \\ -23.0437 & 43.0915 \end{bmatrix},\ Q_{22} = \begin{bmatrix} 72.9823 & 17.2892 \\ 17.2892 & 50.8670 \end{bmatrix},\ Q_{122} = \begin{bmatrix} 81.8514 & 50.3456 \\ 50.3456 & 39.8423 \end{bmatrix},$$

$$Q_{13} = \begin{bmatrix} 93.3250 & 9.8202 \\ 9.8202 & 77.4496 \end{bmatrix},\ Q_{23} = \begin{bmatrix} 61.4088 & -23.0449 \\ -23.0449 & 48.9820 \end{bmatrix},\ Q_{123} = \begin{bmatrix} 80.4472 & 15.3662 \\ 15.3662 & 50.4499 \end{bmatrix}.$$

From Eq. (3.5), we have

$$\Lambda_1 = \begin{bmatrix} 2.0797 & 5.6548 \\ 5.6548 & 15.8965 \end{bmatrix},\ \Lambda_2 = \begin{bmatrix} 7.7627 & -13.0736 \\ -13.0736 & 22.0329 \end{bmatrix},\ \Lambda_3 = \begin{bmatrix} 52.6056 & 23.8213 \\ 23.8213 & 11.1730 \end{bmatrix}$$

and the eigenvalues of them are given below:

$\lambda(\Lambda_1) = 0.0605,\ 17.9157 > 0$, $\lambda(\Lambda_2) = 0.0039,\ 29.7917 > 0$, $\lambda(\Lambda_3) = 0.3201,\ 63.4586 > 0$.

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. As a modified fuzzy control order, the following has been adopted as a feedback theory based on the energy function and LMI optimal stability criteria, which allows researchers to solve this problem and ensure the entire integrated system is in asymptotic stability.

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