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Application of Strain Gradient Elasticity in Analysis of Elastic Properties of Single Walled Carbon Nanotubes

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ABSTRACT

In this paper, the size effect on elastic properties of single- walled nanotubes is evaluated via the strain gradient elasticity approach. For this purpose, rod, torsion bar and Euler- Bernoulli beam models are used. The tension rod model is developed in the present study. The Euler- Bernoulli beam model is utilized and the boundary conditions are modified in the present research. In addition, a model for the rod under torsion is developed. Afterwards, by using the constitutive relation in strain gradient elasticity, the size- dependent elastic properties of carbon nanotube are achieved effectively. The results show that the length of the carbon nanotube is more effective on the Young modulus in comparison with that of on shear modulus and when the length of nanotube decreases, the Young modulus decreases similarly.

KEYWORDS:

Strain Gradient Elasticity, Carbon Nanotube, Size Effect, Elastic Properties.

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1- Introduction

In the last two decades, interest in use of very small scale structures for several purposes has been increased. The Micro- electromechanical systems (MEMS), nano- electromechanical systems (NEMS), biosensors, actuators and nanocomposites are some examples of applications of such small scale structures. The nano-beam (NB) as one of the structures that are used in NEMS can also be employed as an element for mechanical modeling of nanotubes which are used in polymer nanocomposites extensively. To determine the mechanical behavior of nanostructures, as well as the experimental methods and atomistic simulations, the continuum mechanics approach is also available. This approach is computationally less expensive than the former approaches and its formulation is simple. So, it can be employed as an alternative way to simulate the mechanical behavior of nanostructures. Experimental evidences show that when dimensions of the continuum and material length scale parameter are at the same order, size effect cannot be neglected. Due to lack of existing such intrinsic length scales in the classical continuum theory, these experimental observations cannot be captured by this theory. Among the non- classical continuum theories, the strain gradient theory [1] is a theory which, gradients of strain must be considered in addition to the strain in the strain energy density function of the deformable body. Comparison between different models in this area, the simplified strain gradient elasticity is of more practical importance. This stems from its simpler implementation not only because just one internal length is involved but also because of the structure of the governing equations which is dominated by the Laplacian operator. In this research the size effect on elastic properties of carbon nanotube [2] is investigated based on the strain gradient elasticity theory.

2- Methodology

In order to assess the size effect on elastic properties of the carbon nanotube, a simplified strain gradient elasticity theory [3, 4] is employed. The rod, Euler-Bernoulli beam and torsion bar models are used in strain gradient elasticity context to capture the size effects on the elastic behavior of the carbon nanotube. The governing equations and boundary conditions are derived in variational framework and solved by mathematical software Maple 14. In addition, by introducing an effective constitutive equation, the length scale effect on the Young's modulus and shear modulus of carbon nanotube is investigated.

3- Main Contributions

Some of the important achievements of this research are listed as following:

- Introduction of effective constitutive equation in the strain gradient elasticity theory
- Modification of the boundary conditions of beam model by the authors to capture size effect exactly.
- Using a more appropriate beam model than rod model to capture the size effect on the Young's modulus of carbon nanotube.
- Development of governing equation and boundary conditions of torsion bar in strain gradient elasticity framework.

4- Simulation Results

The size dependent Young modulus of a (10, 10) carbon nanotube may be observed in the Fig. 1. The Young modulus of carbon nanotube has been shown for several length based on experimental results and present work. As the length of carbon nanotube increases, its Young modulus increases.

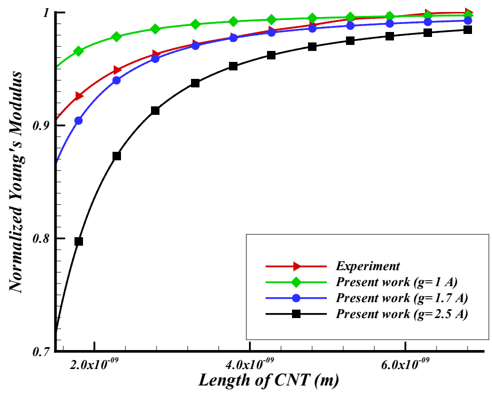

Figure 1. Size dependent Young modulus of carbon nanotube

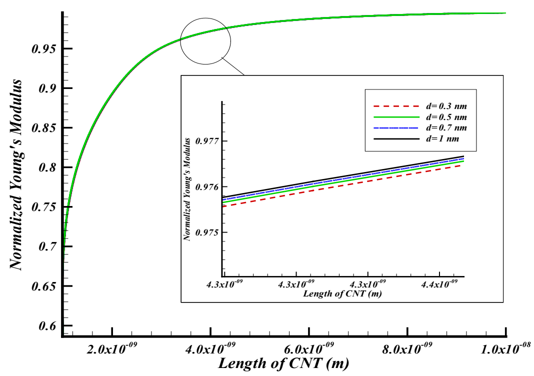

Figure 2. Size dependent Young modulus of carbon nanotube

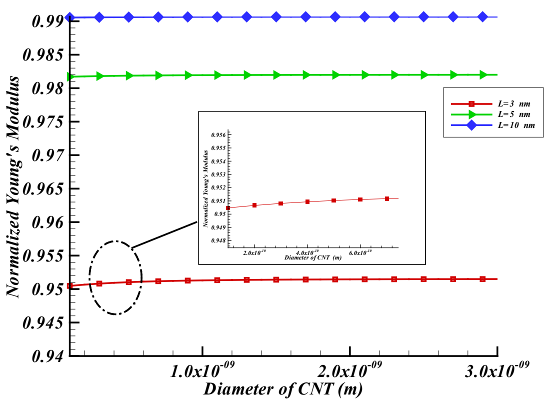

Figure 3. Diameter dependent Young modulus of carbon nanotube for constant lengths

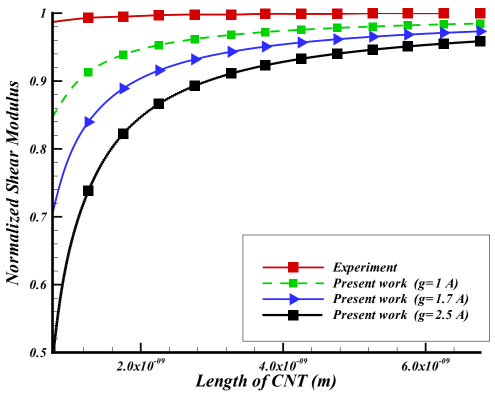

Figure 4. Size dependent shear modulus of carbon nanotube.

On the other hand, length dependent Young modulus of CNT in several diameters has been displayed in Fig. 2. The characteristic length is equal to 1.7 angstrom.
As it can be seen, the diameter has a negligible effect on CNT's Young modulus. It means that the CNTs with different diameter have the similar effect on CNT's Young modulus. Of course for clarifying the diameter effect on Young modulus of CNT, Fig. 3 shows the diameter dependent Young modulus in constant lengths.
As depicted in Fig. 4, the size dependent shear modulus of carbon nanotube has been displayed against different lengths. Experimental results reveal that the length of carbon nanotube is not effective on shear modulus of carbon nanotube. However the present theory predicts significant effects of length on shear modulus.

5- Main References

[1] Mindlin R. D., "Micro- structure in linear elasticity", Archive for Rational Mechanics and Analysis, Vol. 16, pp. 51- 78, 1964.

[2] Iijima S., "Helical microtubules of graphitic carbon", Nature, Vol. 354, pp. 56- 58, 1991.

[3] Aifantis E. C., "On the role of gradients in the localization of deformation and fracture", International Journal of Engineering Science, Vol. 30, pp. 1279- 1299, 1992.

[4] K.A. Lazopoulos, A.K. Lazopoulos, "Bending and buckling of thin strain gradient elastic beams", European Journal of Mechanics - A/Solids, Vol. 29, No. 5, pp. 837- 843, 2010.