Proceedings of the International Conference on Nanotechnology: Fundamentals and Applications
Ottawa, Ontario, Canada, 4-6 August 2010
Paper No. 420

Prediction of Young's Modulus of Perfect and Defective SWCNTs with Various Loading Methods

V. Parvaneh, M. Shariati
Shahrood University of Technology, Department of Mechanical Engineering
Daneshgah Blvd, shahrood, Semnan, Iran
Member of the Young Researchers Club of Azad University of Mashhad
Vali.Parvaneh@gmail.com; mshariati44@gmail.com

ABSTRACT

In this paper, the influence of various vacancy and Stone-Wales defects on the Young's modulus of single walled carbon nanotubes is investigated via a structural model. Dispersion in experimental results is the motivation for this work. Our results show that the type of method used (loading and boundary condition) for the prediction of the Young's modulus of SWCNTs is very important for the results. The effect of different types of defects on the Young's modulus is also studied for zigzag and armchair nanotubes with various aspect ratios (length/diameter). Comparison of our results with those of experimental methods indicates that for the exact prediction of the Young's modulus of SWCNTs, we need to apply the correct conditions.

1 INTRODUCTION

The discovery of carbon nanotubes by Iijima (1991) opened up a new window in nanoscience. Due to the particular mechanical and electrical features of carbon nanotubes, this kind of nanostructure has come under close scrutiny by many researchers in recent decades. A very high Young's modulus and tensile strength combined with low density give these materials excellent mechanical properties. About one year after that, Iijima (1993) predicted the Young's modulus of SWCNTs at about 1 TPa. Then experimental work on the prediction of mechanical properties of SWCNTs increased. Various investigators have conducted experimental research to study the Young's modulus of carbon nanotubes. The Young's modulus can be obtained by different methods. Wong et al. (1997) presented the mean experimental data as 1280 GPa for SWCNTs by the cantilever bending method. Krishnan et al. (1998) found the Young's modulus of SWCNTs to be on average 1250 GPa for SWCNTs. They obtained their results by investigating the thermal vibrations of SWCNTs. Salvatat et al. (1999) and Tombler et al. (2000) reported the Young's modulus of SWCNTs of 810 GPa and 1200 Gpa, respectively, by the three point bending method. Yu et al. (2000) reported the Young's modulus of SWCNT ropes at about 750 GPa by the tension test. Comparison of these results with each other indicates a great amount of scattering between them. One reason for this problem can be defects. It should be noted that the quality of nanotubes used in the experiments have a significant effect on the results and the scatter of the data. Another important reason can be type of method of experimental tests. The most commonly used instrument is atomic force microscopy (AFM), which is used to apply loads to the nanotube in bending and tension tests. The necessity of desirable conditions for experimental tests and limitations in the instruments used are other reasons for the large scatter in experimental data. Many theoretical and numerical models have also been employed for the prediction of the Young's modulus; however, the tension test is used by all of them. Therefore, we will not focus on modeling and simulation results, as dispersion in the results are due to their models and not the type of loading method.

Therefore, this paper investigates the effect of different vacancy and stone-wales defects on the Young's modulus of SWCNTs. In addition to effect of defects, we studied the effect of different loading and boundary conditions. Here, we examine the Young's modulus of SWCNTs by four usual mechanical methods: tension, free-fixed bending, simple-simple bending and fixed-fixed bending.

The model for the carbon nanotubes is an atomistic modeling technique using ABAQUS software. This atomistic modeling technique is the molecular structural mechanics approach, which has been

successfully used for the prediction of the elastic axial buckling of carbon nanotubes under compressive loads (Parvaneh et al., 2009).

2 APPLICATION OF THE STRUCTURAL MODEL SWCNTs

We have proposed a structural mechanics method to model the carbon nanotubes. The detailed derivation procedure for the formulation and other features of this model can be found in our previous work [20]. Here, we take $E = 1170GPa$ GPa and $\nu = 0.19$ for the Young's modulus and Poisson's ratio of single-walled carbon nanotubes, respectively. As shown in our previous work, we used $k_r = 8100Nm$, $k_\theta = 14.22NmRad$, $k_\phi = k_\tau = 9.04nm$, which are consistent with the values reported in the literature. This structural model was successfully used for predicting the mechanical properties and axial buckling behavior of single-walled carbon nanotubes. It is employed here for predicting the Young's modulus of single-walled carbon nanotubes.

3 FOUR METHODS FOR YOUNG'S MODULUS OF PERFECT SWCNTs

The tension test is one of the well-known methods for the prediction of the Young's modulus of materials. To find the exact Young's modulus of a circular shell on the macroscale, we usually construct a standard segment from materials and test it instead of circular shell. However, we cannot apply this method for materials on the nanoscale, such as carbon nanotubes. Therefore, in the tension test for a carbon nanotube, we stretch the carbon nanotubes from tow ends. Here, we fix the tow plane at the ends of nanotube and apply an unaxial force to the center of the tow planes (see Fig. 1(a)).

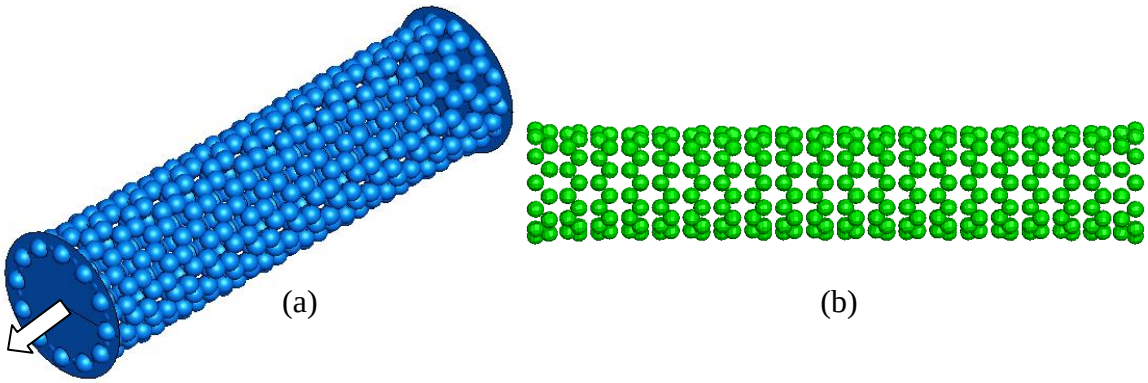

Fig. 1: Boundary and loading conditions of the structural model of SWCNTs (a) and deformed configuration of zigzag (12,0) subjected to tension (b).

We performed the tension test on perfect zigzag (12,0) and armchair (7,7) SWCNTs with various aspect ratios (L/d). Fig. 1(b) shows the deformed configuration of a perfect zigzag (12,0) nanotube after the tension test.

We also obtained the Young's modulus by bending tests. Three types of bending tests are shown in Fig. 2. For short lengths of nanotubes, local bending will occur (see Fig. 2(b)), and for longer nanotubes, global bending will occur (see Fig. 2(c) and (d)). The Young's modulus of a SWCNT from free-fixed, fixed-fixed and simple-simple bending tests is obtained from continuum mechanics Eq. (1)-(3), respectively:

$$E = \frac{FL^3}{6\delta I} \tag{1}$$

$$E=\frac{5FL^3}{96\delta I} \tag{2}$$

$$E=\frac{FL^3}{48\delta I} \tag{3}$$

where L, I, F and δ are the length of the nanotube, the cross-sectional moment of inertia, the applied force and the displacement of the center of the nanotube, respectively. The effective wall thickness of SWCNTs is 0.34 nm. These three equations are obtained from continuum mechanics theories and utilized for continuum beams.

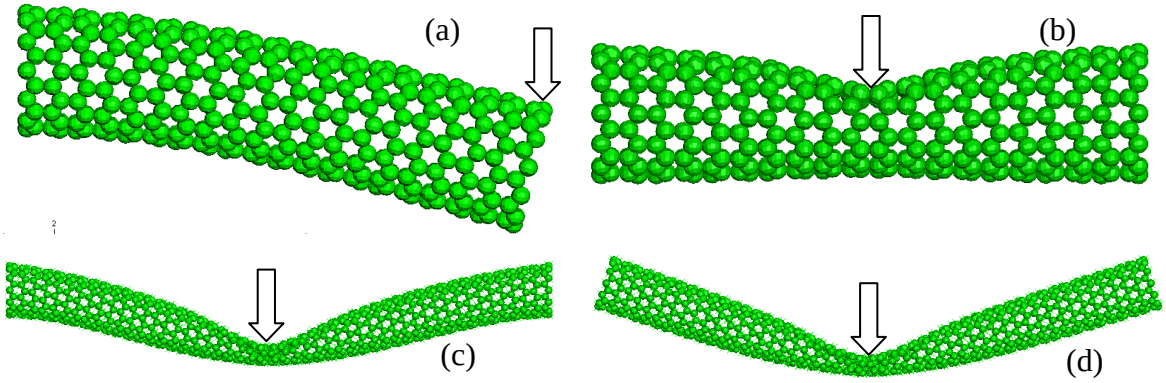

Fig. 2: Deformed shape of free-fixed zigzag (12,0) subjected to bending (a), local bending of fixed-fixed zigzag (b), global bending of fixed-fixed zigzag (c), global bending of simple-simple zigzag (d).

The Young's modulus is found by four mechanical methods for perfect nanotubes with different aspect ratios and compared with each other (see Fig. 3).

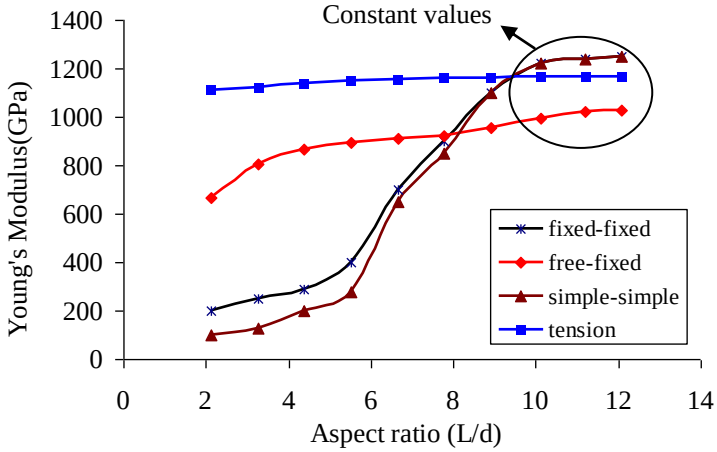

Fig. 3: Young's modulus of single-walled carbon nanotube as a function of nanotube aspect ratio.

It is seen from Fig. 3 that the Young's modulus for both armchair and zigzag nanotubes increases with increasing aspect ratio and approaches a constant value. This increase is lacking for the tension test; however, it is present in free-fixed bending and much more so in simple-simple and fixed-fixed bending. For more accurate in experimental tests, we must use sufficiently long nanotubes. The comparison of the Young's modulus obtained by the four methods indicates that the predicted Young's modulus from the tension test results for different aspect ratios is approximately, constant; the Young's modulus of each material is constant and does not depend on geometrical parameters, and hence it seems that the tension test presents the best results. However, with increasing length of nanotube, the predicted Young's

modulus by the three bending tests will increase and approach a constant value. For sufficiently long nanotubes, the minimum predicted value for the Young's modulus by these four methods is dependent on free-fixed bending, and the maximum value depends on simple-simple and fixed-fixed bending. It appears that the best method for the prediction of the Young's modulus of carbon nanotubes is the tension test because in addition to the above noted advantage, the predicted Young's modulus by this method is moderate.

From a length of 5 nm and up, we have seen that the Young's modulus increases greatly for the fixed-fixed and simple-simple bending methods. This change is due to the variation of the mode shapes from local bending to global bending (see Fig. 2). Eq(2) and (3) answer exactly for global bending. Hence, for the prediction of the Young's modulus of carbon nanotubes by bending methods, we have to consider nanotubes with aspect ratios of up to 8 to obtain more exact results.

4 YOUNG'S MODULUS OF DEFECTIVE SWCNTs

Due to the restrictions of CNT manufacturing, production of perfect nanotubes is very hard, and the percentage of those is very low compared to the percentage of defective nanotubes. Vacancies result from missing carbon atoms in the CNT walls. This can happen when CNTs are subjected to irradiation. The types of vacancy defects for the study of defects in carbon nanotubes are illustrated in Fig. 4. The defects included are single vacancies, double vacancies and triple vacancies. All of the defects are situated in the middle of the nanotube.

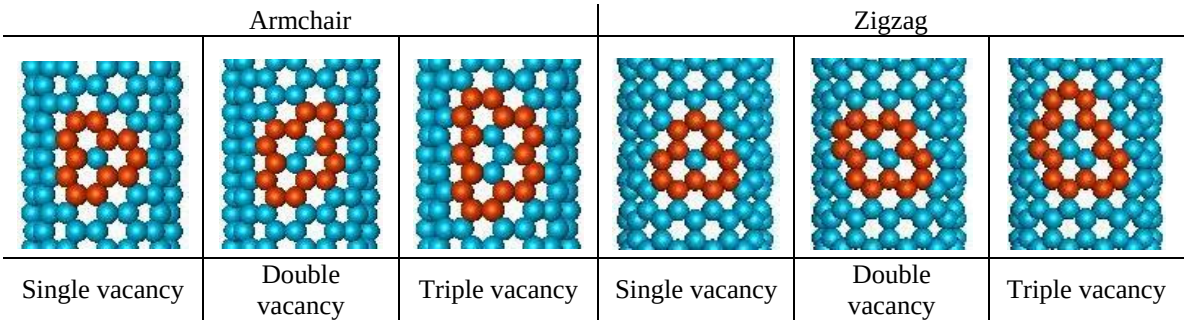

Fig. 4: Different vacancy defects used in analysis.

For zigzag (12,0) and armchair (7,7) nanotubes with vacancy defects under tension, the Young's modulus as a function of the nanotube length is shown in Fig. 5. It is seen that the influence of vacancy defects on the Young's modulus for both zigzag and armchair nanotubes decreases with increasing nanotube length, and these defects have more effect on the Young's modulus at short lengths. Furthermore, zigzag nanotubes are more sensitive to variations of length at short lengths. The main reason for this is the different orientation of the vacancy defects (see Fig. 4). Another reason for this difference is due to orientation of the C-C bonds for zigzag CNTs that are in the load direction. Therefore, distribution of load on the carbon atoms for zigzag and armchair CNTs is uniform in the circumferential and axial direction, respectively.

Fig. 6 shows the deformed configuration of nanotube with vacancy defects after free-fixed bending tests for zigzag and armchair nanotubes. As observe in Fig. 6, vacancy defects cause a nick at the defect location.

In Fig. 7, the comparison of the Young's modulus of perfect and defective SWCNTs with vacancy defects by the free-fixed bending test is illustrated. It can be observed that for the same length and diameter, the Young's modulus of the armchair nanotube is higher than that of the zigzag nanotube. Furthermore, it can be seen that values of the Young's modulus are more sensitive to vacancy defects with shorter tubes. With increasing nanotube length, the influence of vacancy defects decreases.

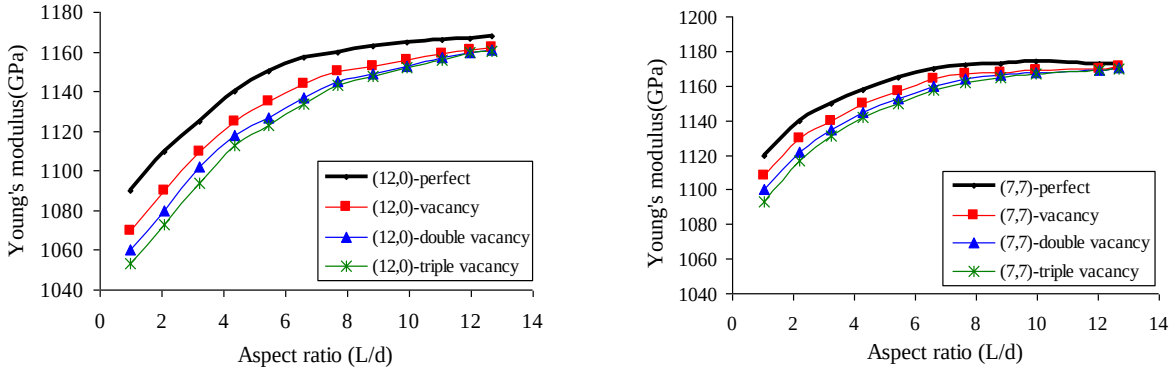

Fig. 5: Influence of vacancy defects on the Young's modulus with variation of nanotube length by tension test.

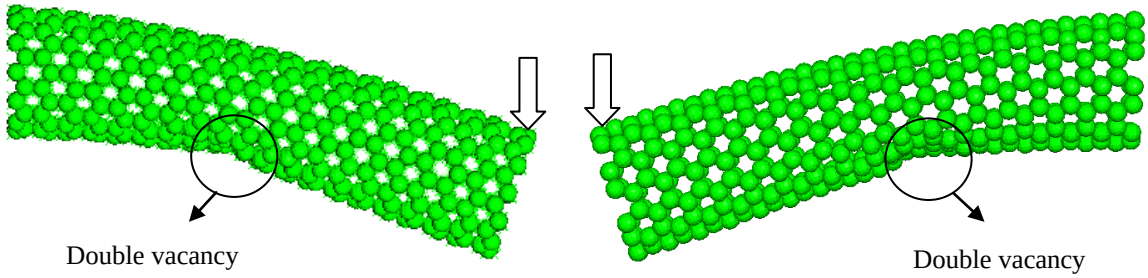

Fig. 6: Deformed configuration of defective zigzag (12,0) (a) and armchair (7,7) (b) nanotubes with one double vacancy subjected to free-fixed bending.

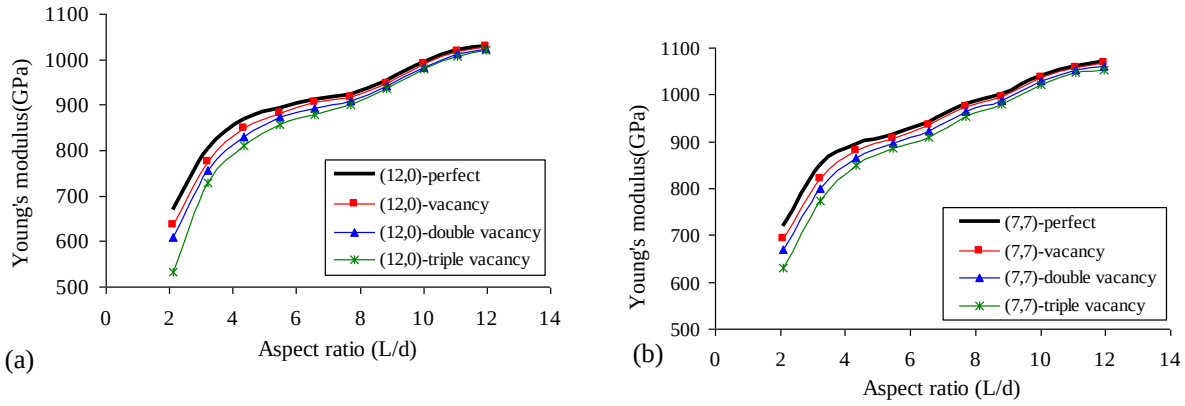

Fig. 7: Influence of vacancy defects on the Young's modulus with variation of nanotube length by the free-fixed test.

Stone-Wales defects in carbon nanotubes are generated under the certain conditions. Stone and Wales showed that a dipole consisting of a pair of 5-7 rings can be created by rotating the C-C bond in a hexagonal network by 90o. Here, we suppose that an initial Stone-Wales defect exists on the nanotube before the tension test (see Fig. 8). This defect is in the middle of the nanotube.

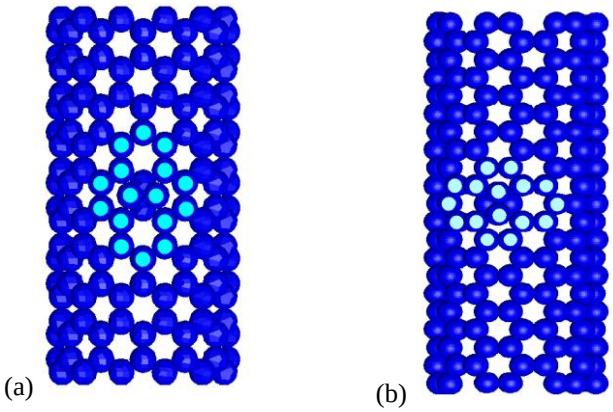

Fig. 8: Critical buckling loads of defective nanotubes with various aspect ratios for (a) Zigzag and (b) Armchair.

Table 1 summarizes the Young's moduli obtained from perfect nanotubes and compares them with those of nanotubes with Stone-Wales defects. The Young's modulus is found for nanotubes with Stone-Wales defects with different diameters and lengths by the tension and free-fixed bending tests. Generally, the effect of Stone-Wales defects on the decrease of the Young's modulus is much lower than vacancy defects, and these weak defects do not have a significant effect on the Young's modulus of the nanotubes.

Table 1. Parameters for molecular mechanics potentials.

		Tension		**Free-Fixed bending**	
Tube size (nm)		Young's modulus (TPa)			
Chirality	Length	No defect	Stone-wales	No defect	Stone-wales
(12,0)	4.118	1140	1132	869	860
(12,0)	12.354	1167	1165	1030	1029
(7,7)	4.058	1158	1155	895	891
(7,7)	12.174	1173	1172	1072	1072
(16,0)	4.118	1148	1144	875	870
(16,0)	12.354	1169	1168	1033	1032
(9,9)	4.058	1165	1163	902	898
(9,9)	12.174	1174	1174	1075	1073
(22,0)	4.118	1150	1149	879	878
(22,0)	12.354	1170	1170	1034	1034
(13,13)	4.058	1166	1166	903	901
(13,13)	12.174	1175	1175	1077	1077

CONCLUSION

Various methods for the prediction of the Young's modulus of SWCNTs have been investigated via the structural mechanics model. For all of the experimental tests that were used for the prediction of the Young's modulus, we needed to select a sufficiently long nanotube. This option is more sensitive for fixed-fixed and simple-simple bending tests. The best method for the prediction of the Young's modulus

of single-walled carbon nanotubes is the tension test. Defects do not have a significant effect on the Young's modulus of sufficiently long SWCNTs. However, for nanotubes with shorter lengths, this effect is much greater, and armchair nanotubes are more sensitive to defects than zigzag nanotubes in general.

REFERENCES

Iijima S. (1991). Helical microtubes of graphitic .carbon Nature, 354, 56–58**.**

Iijima S., Ichlhashi T. (1993). Single-shell carbon nanotubes of 1-nm diameter. Nature, 363, 603–605.

Krishnan A., Dujardin E., Ebbesen T.W., Yianilos P.N., Treacy MM.J. (1998). Young's modulus of single-walled nanotubes. Phys Rev B, 58, 14013-9.

Parvaneh V., Shariati M., Majd Sabeti A.M. (2009). Investigation of defects effects on the buckling behavior of SWCNTs via a structural mechanics approach. European Journal of Mechanics A/Solid, 28, 1072–1078.

Tombler T.W., Zhou C., Alexseyev L., Kong J., Dai H., Liu L., Jayanthi C.S., Tang M., Wu S. (2000). Reversible electromechanical characteristics of carbon nanotbues under local-probe manipulation. Nature, 405, 769-772.

Wong E.W., Sheehan P.E., Lieber C.M. (1997). Nanobeam mechanics: elasticity, strength, and toughness of nanorods and nanotubes. Science 277, 1971–1975.

Salvetat J., Bonard J., Thomson N.H., Kulik A.J., Forro L., Benoit W., Zuppiroli L. (1999). Mechanical properties of carbon nanotubes. Applied Physics A, 69, 255-260.

Yu M., Files B., Arepalli S., Ruoff R. (2000). Tensile loading of ropes of single wall carbon nanotubes and their mechanical properties. Physical Review Letters, 84, 5552-5555.