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Equivalent beam model of single walled carbon nanotube with imperfections

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Abstract. The presented paper is a continuation to authors' previous work on numerical modelling of carbon nanotubes (CNTs) and CNT reinforced nanocomposite materials. One of the numerical method approach for CNT modelling is based on structural mechanics. Proposed method is proven and effective, but has some disadvantages when it is used in nanocomposite material FEM modelling. In addition, different defects within CNTs structure, as well as the waviness of CNTs, greatly influence the mechanical properties of CNTs. The paper at hand proposes the equivalent beam model for modelling the single walled carbon nanotubes (SWNT), straight and waved, with vacancy defects within structure.

1. Introduction

A great deal of scientific papers, with both theoretical and experimental research on single and multi walled carbon nanotubes (SWNT; MWNT), has been published [1, 2, 3]. Common conclusion of all the researches is that CNTs possess extraordinary material properties, which makes them an excellent choice as a composite material reinforcement [4, 5]. Their nano size is a source of a lot of problems when it comes to investigating CNTs mechanical properties, so numerical methods and computer assisted modelling emerges as logical solutions for given quest. One of the tested and proven numerical method is based on structural mechanics. In proposed method, since the CNT is basically a space frame structure, or molecule, consisting from carbon atoms and covalent bonds, the covalent bonds are replaced with the beam finite elements, and atoms with nodes. [6, 7, 8]. That gives approximately 2350 finite elements per one SWNT (with the length around 13,77 nm), depending on CNT pattern. The problem arises when this CNT model is to be used in nanocomposite modelling where, in addition to CNT finite model, one has to model matrix of nanocomposite and matrix – reinforcement (CNT) interaction. The number of finite elements in such nanocomposite model arises drastically, due to interaction modelling by using nonlinear rod elements [8, 9]. Multiscale modelling methods are smooth way to overcome this issue, but nevertheless, the proposed equivalent beam model of CNT can also be an effective solution. Early research on CNTs was directed toward determination of mechanical properties of ideally shaped CNTs [10, 11, 12], but more exact research detected that SWNT and MWNT carbon nanotubes rarely come in ideal form and without defects. Regardless of the manner of production control and methods, CNTs are usually waved [13, 14], and studies have shown that the waviness of the nanotube has an influence on the final mechanical properties of CNTs, namely longitudinal elastic modulus, and, thus, nanocomposite materials [15, 16, 17]. Another common problem in nanotube structure is appearance of various defects [18, 19, 20], which can occur either naturally or artificially. The impact of mentioned imperfections on longitudinal elastic moduli of SWNT and DWNT was investigated in authors' previous work [21], and those



obtained results are basis for determination of elastic moduli for proposed equivalent SWNT beam model, presented in this paper. The armchair (5, 5) and zig-zag (9, 0) pattern of straight and waved SWNTs, with different vacancy defects are considered.

2. SWNT examples

Carbon nanotubes have very high aspect ratio (diameter/length ratio), with diameter in order of nanometers and length in micrometers. High aspect ratio leads to waved shape of CNTs, which is experimentally proved [18, 19], and to small bending stiffness. Waviness of CNTs is in literature defined with the waviness ratio w [22], as ratio between wave amplitude and wavelength. However, mechanical properties of CNTs are affected also by various defects within nanotube structure, which can occur either naturally or artificially. The incomplete bonding defects, i.e. vacancies or missing atoms in CNT structure, are influential when it comes to final mechanical properties of carbon nanotubes, especially longitudinal elastic modulus [21]. Table 1. shows the degradation of longitudinal elastic modulus value, with the increase of the both, the waviness ratio w and the number of vacancies within CNT structure, for both patterns; armchair and zig-zag. These results are obtained from authors' previous work [21]. The CNT models used in aforementioned paper are briefly described as follows. Armchair (5, 5) and zig-zag (9, 0) patterns are selected for SWNT, with similar diameter (0,678nm – 0,695nm) and aspect ratio (20,2). All CNTs are modelled as a space frame structure (atoms replaced by nodes, covalent bonds with the beam finite elements [6, 7, 8]). Using eigenvalue analysis, the waved shape of the nanotubes were obtained. Four SWNT models were prepared and used, straight and three waved, with waviness ratios 0.03; 0.05 and 0.08, as shown in figure 1.

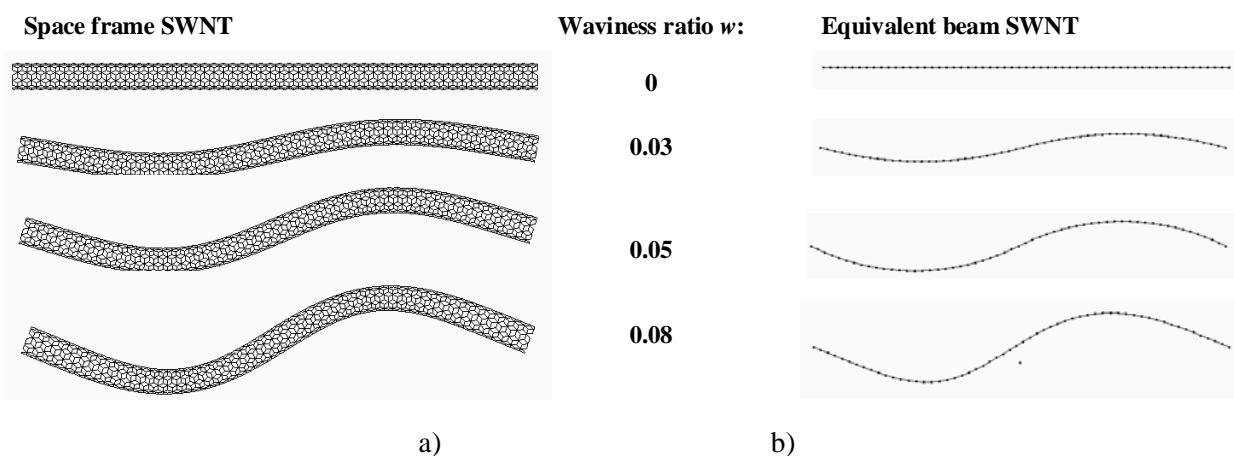


Figure 1. Examples of used SWNT models.

Vacancies in SWNTs are introduced by removing one node and corresponding three beam elements. Respectively, the given percentage of missing atoms (0,1%, 0,5%, 1%, 2%, 5%, 10%), randomly selected, were removed from SWNTs structure. To determine the elastic modulus, an axial loading case was used, with 1 nN axial force used in all examples. The longitudinal elastic modulus was obtained using classical term $E = (F \cdot l / A \cdot \Delta l)$, where l represents nanotube length and Δl the elongation obtained from FEM analysis. The obtained results are shown in the table 1. The results for straight SWNT are the basis for modelling the SWNTs using equivalent beam approach. SWNT models with same waviness ratio were prepared, but using only beam finite elements which represent SWNT geometry (Fig 1b.). The beam finite element property was adjusted and prepared in the manner that they coincide with carbon nanotube properties, i.e. cross sectional area and moment of inertia. The data obtained using space frame approach, for straight SWNT, namely the elastic modulus values, were used as relevant in defining the material characteristics of beam finite element property. The number of finite elements per one SWNT drops to only 57 elements, as opposed to 2350 finite

elements in space frame model of SWNT. After the conducted analysis, same axial loading case was used to obtain the values for the longitudinal elastic moduli of equivalent beam SWNT model, and those results are given in table 2. The analysis was carried out for armchair and zig-zag pattern, with the same waviness ratio and vacancies percentage.

3. Results

Results for longitudinal elastic modulus obtained from aforementioned examples are given in following tables and figures. Tables 1. and 2. show the results for armchair and zig-zag SWNT, space frame approach and equivalent beam approach, respectively. As it is been shown before, there is a noticeable drop of longitudinal elastic modulus with the increase of the waviness ratio of the nanotube, regardless of the CNT type and pattern. The value of elastic modulus also decreases with the increase of the vacancies within the same waviness ratio of the CNT, but is practically unaffected when percentage of defects is less than 1%. The same behaviour pattern can be observed in equivalent beam approach models, figure 2. and 3.

Table 1. Results for space frame models of SWNT

Vacancy %:	Longitudinal elastic modulus E , GPa							
	Waviness ratio, w (armchair):				Waviness ratio, w (zig-zag):			
	0	0.03	0.05	0.08	0	0.03	0.05	0.08
No defects	1048.76	341.58	135.09	74.27	1030.99	349.11	139.97	77.45
0.1%	1008.82	335.58	132.74	72.96	987.36	342.38	138.77	73.05
0.5%	979.79	316.59	127.16	71.98	918.42	328.33	129.49	74.78
1%	908.78	313.61	126.50	69.89	848.07	310.91	124.27	73.59
2%	796.56	285.31	117.67	60.25	818.34	299.12	97.38	56.66
5%	662.10	219.99	76.94	47.99	446.47	87.64	103.91	47.93
10%	146.87	74.42	59.98	13.91	282.99	60.26	36.85	18.77

Table 2. Results for equivalent beam models of SWNT

Vacancy %:	Longitudinal elastic modulus E , GPa							
	Waviness ratio, w (armchair):				Waviness ratio, w (zig-zag):			
	0	0.03	0.05	0.08	0	0.03	0.05	0.08
No defects	1048.76	375.87	166.57	97.44	1030.98	381.31	169.69	99.22
0.1%	1008.82	361.56	160.23	93.73	987.36	365.18	162.51	95.02
0.5%	979.79	351.16	155.62	91.03	918.42	339.68	151.16	88.39
1%	908.78	325.71	144.18	84.43	848.07	313.66	139.58	81.62
2%	796.56	285.49	126.51	74.01	818.34	302.66	134.69	78.75
5%	662.10	237.29	105.16	61.52	446.47	165.13	73.48	42.97
10%	146.87	52.64	23.33	13.65	282.97	104.66	46.57	27.23

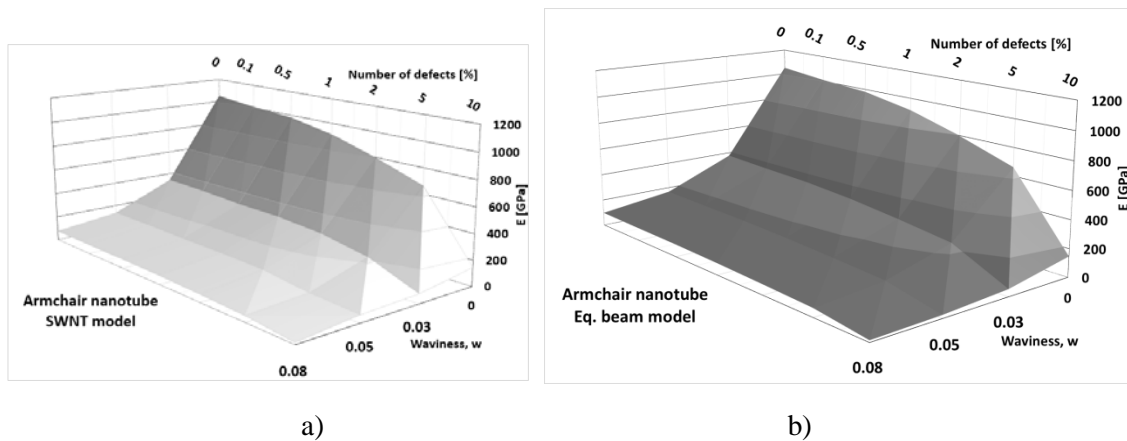


Figure 2. Change of: elastic modulus/waviness ratio/number of defects for Armchair SWNT: space frame model (a), equivalent beam model (b).

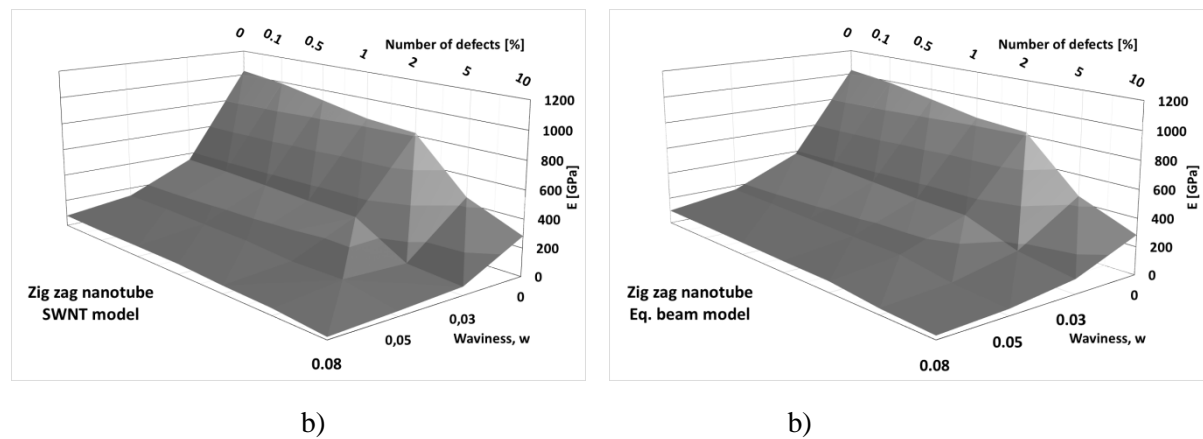


Figure 3. Change of: elastic modulus/waviness ratio/number of defects for Zig-zag SWNT: space frame model (a), equivalent beam model (b).

4. Conclusions

The equivalent beam modelling of single walled carbon nanotube approach is shown and analysed in this paper, on finite element model of armchair and zig-zag SWNT pattern. This was done on nanotubes with different waviness ratio and with different number of vacancies within structure. The main goal and idea was to replace the space frame model of SWNT with simpler, equivalent beam model, but to retain all of the characteristics and benefits of space frame model of SWNT, or better said to retain all of the characteristics of the real carbon nanotube. The obtained results confirm the validity of equivalent beam model, but it has to be emphasized that presented models are adequate for small strain problems. Presented equivalent beam model will be useful in future research on theoretical modelling of nanocomposite materials, reinforced with SWNT, since the number of finite elements in the nanocomposite model will be significantly lesser, and thus, the new approaches offer.

Acknowledgments

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References

- [1] Xie S, Li W, Pan Z, Chang B, Sun L 2000 *J Phys Chem Solids* **61** 1153-1158

- [2] Ruoff RS, Qian D, Liu WK 2003 *Physique* **4** 993-1008
- [3] Wan H, Delale F 2010 *Meccanica* **45** 43-51
- [4] Tserpes K I, Papanikos P, Labeas G, Pantelakis S G 2008 *Theoretical and Applied Fracture Mechanics* **49** 51-60
- [5] Murarescu M, Dima D, Andrei G, Ciriumaru A 2011 *Annals of DAAAM for 2011 & Proceedings of 22nd International DAAAM Symposium* **22** 925-6
- [6] Brcic M, Canadija M, Brnic J, Lanc D, Krscanski S, Vukelic G 2009 *Estonian Journal of Engineering* **15** 77-86
- [7] Canadija M, Brcic M, Brnic J 2013 *Review on Advanced Materials Science* **33** 1-6
- [8] Brcic M, Canadija M, Brnic J 2013 *Meccanica* **48** 2209-20
- [9] Canadija M, Brcic M, Brnic J 2017 *Meccanica* **53** 1655-1668
- [10] Fisher F T, Bradshaw R D, Brinson L C 2002 *Applied Physics Letters* **80** 4647-49
- [11] Fisher F T, Bradshaw R D, Brinson L C 2003 *Composites Science and Technology* **63** 1689-1703
- [12] Bradshaw R D, Fisher F T, Brinson L C 2003 *Composites Science and Technology* **63** 1705-22
- [13] Ebbesen T, Takada T 1995 *Carbon* **33** 973-8
- [14] Shokrieh M M, Rafiee R 2010 *Composite Structure* **92** 647-52
- [15] Jiang L Y, Huang Y, Jiang H, Ravichandran G, Gao H, Hwang K C 2006 *Journal of the Mechanics and Physics of Solids* **54** 2436-52
- [16] Tan H, Jiang L Y, Huang Y, Liu B, Hwang K C 2007 *Composite Science and Technology* **67** 2941-46
- [17] Qian D, Wagner G J, Liu W K, Yu M, Ruoff R S 2002 *Appl. Mech. Rev* **55** 495-533
- [18] Shaffer M S P, Windle A H 1999 *Adv. Mater.* **11** 937-41
- [19] Vigolo B, Penicaud A, Coulon C, Sauder C, Pailler R, Journet C, Bernier P, Poulin P 2000 *Science* **290** 1331-34
- [20] Patel A M, Joshi A Y 2016 *Procedia Technology* **23** 122-9
- [21] Brcic M, Canadija M, Brnic J 2018 *IOP Conf. Series: Materials Science and Engineering* **378**
- [22] Farsadi M, Ochsner A, Rahmandoust M 2012 *Journal of Composite Materials* **47** 1-10