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Influence of Waviness and Vacancy Defects on Carbon Nanotubes Properties

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Abstract

Previous and present theoretical and experimental research of polymer and other composites have shown that carbon nanotubes, acting as an reinfocements, significantly affect the final mechanical properties of aforementioned composites, thanks to its exceptional mechanical properties. However, the properties of carbon nanotube can be affected by the shape of nanotube, as well as various vacancy deffects within the structure of carbon nanotube. Thus, the waviness and the vacancy deffects decreases the final properties of nanocomposite structures. In this paper, the properties of straight and waved carbon nanotube are compared, on examples with different waviness factor, using the finite element method. Also, different vacancy defects are considered on the same straight and waved nanotube models.

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Keywords: carbon nanotube; waviness; vacancy defect

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1. Introduction

Since the discovery of the carbon nanotubes [1], many researchers have attempted to find out their properties and characteristics, either experimentally [2 - 5] or theoretically [6 - 11]. A common conclusion is that carbon nanotubes possess extraordinary mechanical, thermal and electric properties, thus, they are a logical choice as an improvement in composite materials – nanocomoposites, either to improve mechanical properties of composite, due to their extremely high tensile strength and elasticity modulus [12], or to improve electrical conductivity [13]. Because of their nano size, it is very difficult to conduct experimental studies of carbon nanotubes and nanocomposite materials,

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therefore the computer multiscale modelling and numerical methods emerges as a logical solution. Considering numerical approaches, nanotubes have been modelled separately in two different systems of mechanics, molecular dynamics [8, 11, 14 - 16] and structural mechanics, which is based on the substitution of covalent bonds between the atoms with nodes and beam finite elements. Detailed overview and description of the modelling of nanotubes and multiscale modelling methods of nanocomposites is given in author’s previous works [17 - 19]. The reader is referred to these publications, thus in this paper the attention will not be dedicated to the modelling of carbon nanotubes.

Most of the research on mechanical properties of carbon nanotubes are conducted on ideal model of nanotube [20 - 23]. But carbon nanotubes rarely come in ideal form. They are usually waved, regardless of the manner of production control [24, 25]. Studies have shown that the waviness of the nanotube has an influence on the final mechanical properties of nanocomposite materials [26 - 28]. Also, a common problem in nanotube structure is appearance of vacancy defects [29, 30], which can occur either naturally, i.e. rehybridization, or artificially. It is, therefore, very interesting to study the impact of vacancies and waviness of nanotubes on their mechanical properties, specifically on the elastic modulus, because it eventually leads to decrease of final mechanical properties of nanocomposites. Change of elastic moduli of the carbon nanotube is given in this paper, shown on several examples of carbon nanotubes, with different waviness and vacancy defects.

2. Waviness and vacancy defects

As mentioned before, the carbon nanotubes as a reinforcement in the composite materials significantly affect the final mechanical properties of the nanocomposites, due to its exceptional properties. However, in several papers [31, 32] only the slightly improvement of the nanocomposite properties, reinforced with the carbon nanotubes, has been reported. The reason for this is weak load transfer from the composite matrix to the reinforcement, or better said, weak bond between matrix and the reinforcement, i.e. nanotube, since this bond is established through weak van der Waals bonds [33, 34]. Additional reasons are the waviness of carbon nanotubes and appearance of various defects in nanotube structure.

Experiments have shown that carbon nanotubes within nanocomposites are mainly waved [35, 36]. This can be explained by the fact that nanotubes have very small bending stiffness, due to large aspect ratio, i.e. diameter in order of nanometers and length in order of micrometer. Waviness of the nanotube is in the literature defined with the waviness ratio w [37]:

$$w = \frac{a}{l} \tag{1}$$

where a represents wave amplitude and l wavelength, as shown in Fig. 1.

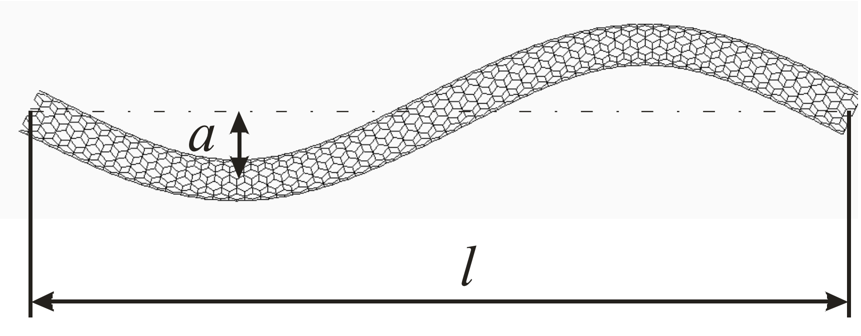

Fig. 1. Definition of the waviness ratio of the nanotube.

Apart from waviness, various defects, such as vacancies, metastable atoms, pentagons, heptagons, heterogeneous atoms, distortion, etc. [38, 39] can appear inside nanotube structure. Vacancies, or missing atoms, greatly reduce strength of the nanotube. Such defects can occur due to the ionic radiation, absorption of electrons or specific production method [40].

3. Examples and results

Influence of waviness and vacancy defects on elastic modulus of carbon nanotube in this paper is shown on finite element model of single walled carbon nanotube, armchair (5, 5) pattern, with diameter 0,679 nm and aspect ratio (length/diameter) 20,2. The nanotube is modelled as a space frame structure, where the atoms are replaced with nodes, and covalent bond with beam finite elements [17 - 19]. There are 1120 nodes and 1670 beam elements in one model of nanotube.

An axially loaded cantilever nanotube model was used to determine the elastic modulus, and 1 nN axial force was used in all examples. The longitudinal elastic modulus was obtained using classical term:

$$E = \frac{F \cdot l}{A \cdot \Delta l} \tag{2}$$

where l represents nanotube length (13,65 – 13,7 nm), A is nanotube's cross section area (0,715 nm^2), and Δl longitudinal elongation.

In relation to term (1), five models of nanotube have been prepared, with different waviness ratio, i.e. four waved nanotube and one straight (w = 0), as shown in Fig. 2. Waved shape of nanotube was prepared using eigenvalue analysis, with different eigenvalue parameters.

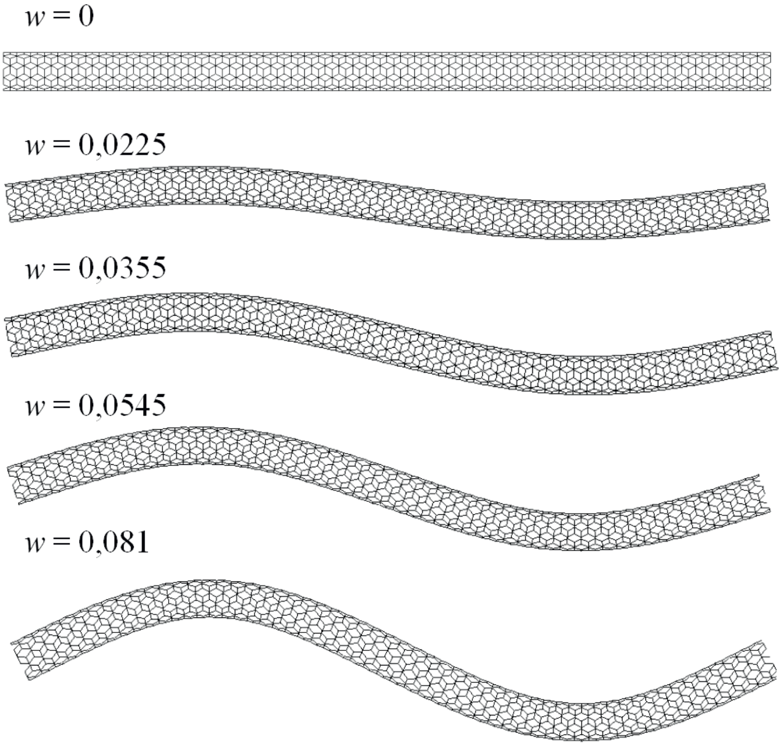

Fig. 2. Examples of waved nanotubes.

Vacancies in nanotube model are obtained by deleting one node and three beam elements from structure. Three different cases of vacancy defects have been prepared, as follows. In first case the vacancies are prepared as shown in Fig. 3., to show the change of elastic modulus versus position of the vacancy.

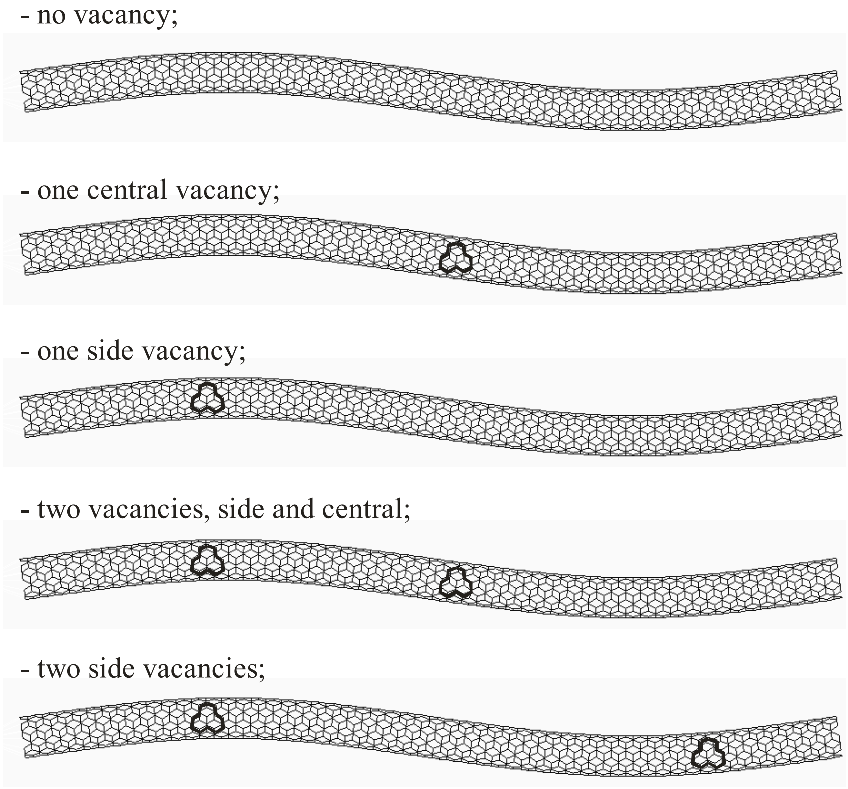

Fig. 3. Vacancy layout in carbon nanotube.

In addition to first case, in the second vacancy case, the given percentage of randomly selected atoms, i.e. nodes (0,1%, 0,5%, 1%, 2%, 5% and 10%) were removed from the nanotube structure. Since vacancies are one of the reason of nanotube waviness, another case of vacancy defects is presented, in which 1 to 8 atoms were removed from the position with maximum curvature at the internal side of the carbon nanotube, Fig. 4. The remaining part of the nanotube is defect free. The latter vacancy defect case was implemented only on the model with waviness ratio 0,0545.

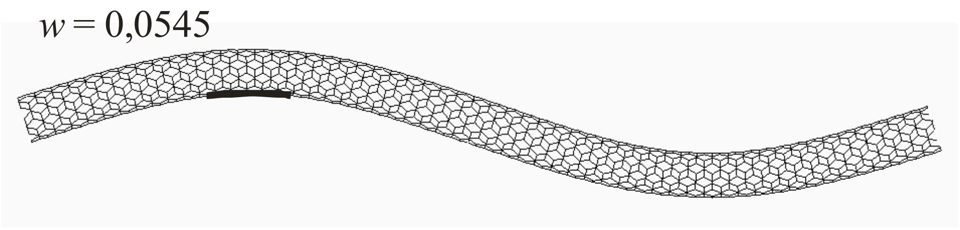

Fig. 4. Position of 1 to 8 vacancy defect in waved nanotube, marked with black line.

Obtained results for longitudinal elastic modulus are given in tables 1 and 2, and in Fig. 5., for corresponding vacancy case. As expected, there is notable drop in elastic modulus value with the increase of the waviness of nanotube. On the other hand, value of elastic modulus also decreases with the increase of the vacancies (from 0,1% to 10%) within the same waviness ratio of the nanotube.

Table 1. Results for first vacancy case.

Longitudinal elastic modulus *E*, GPa					
	Waviness ratio, w:				
Vacancy:	0	0,0225	0,035	0,0545	0,081
No vacancy	1069,42	530,24	187,05	126,36	86,75
1 central vacancy	1040,51	515,91	185,95	125,53	85,21
1 side vacancy	1040,51	515,91	186,50	125,86	85,21
2 vacancies, central and side	1018,49	513,14	185,77	125,36	84,83
2 side vacancies	1018,49	513,14	185,68	125,39	84,94

Table 2. Results for second vacancy case.

Longitudinal elastic modulus *E*, GPa					
	Waviness ratio, w:				
Vacancy percentage:	0	0,0225	0,035	0,0545	0,081
0,1%	1040,51	525,85	183,45	121,52	82,267
0,5%	997,38	534,69	163,06	121,52	79,52
1%	912,29	420,45	175,03	112,23	82,26
2%	844,27	420,45	157,67	102,03	74,55
5%	585,09	329,68	106,58	62,97	53,61
10%	185,09	167,44	23,67	33,53	7,18

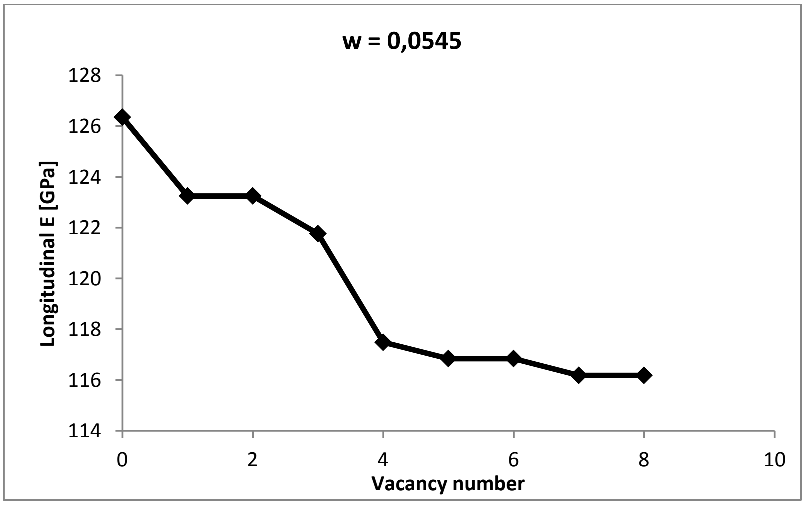

Fig. 5. Results for third vacancy case.

Conclusion

Carbon nanotubes are logical and quality choice as a reinforcement in the nanocomposite materials, due to their excellent mechanical properties. However, because of various causes during production, as well as the geometric characteristics, they come in waved form, with a variety of defects in the structure. Waviness and defects greatly reduce their properties, which ultimately leads to a small improvement of final mechanical properties of nanocomposites. Influence of aforementioned imperfections on nanotube properties, is shown on change of elastic modulus of finite element model of carbon nanotube, with different waviness ratio and different vacancy defects. Thus, the longitudinal elastic modulus of the straight carbon nanotube decreases with increase of the waviness ratio, which is most pronounced in the nanotubes without defects (from 1069 GPa to 86 GPa, 92%). Small decline of elastic modulus is noticeable with the increase of vacancies in the nanotubes with same waviness ratio, from Tab. 1, but with drastic increase of vacancies, a drastic decrease of elastic modulus, within nanotubes with same waviness ratio, can be noticed (Tab. 2.). Irregularities in values of elastic modulus in Tab. 2. can be attributed to randomly positioned vacancies in each particular example, i.e. analysis. Fig. 5. shows change of elastic modulus if vacancies accumulate on specific position in nanotube structure. It should also be noted that values of elastic modulus match in the examples with the same waviness ratio and the same number of vacancies, and from the examples with 1 or 2 vacancies it is possible to conclude that position of the defect doesn't affect the elastic modulus (Tab. 1.).

Acknowledgements

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