Original Article: Investigation of Behavior and Analysis of Mechanical Properties of Carbon Nanotubes under Different Loads

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ABSTRACT

In this research, the behavior and mechanical properties of carbon nanotubes under different loads (tensile and torsional) were investigated using finite element method with SOLIDWORKS Simulation software. Examination of carbon nanotubes by selecting the wrong element and large size of the elements leads to high error in the model and in contrast to the high mesh density increases the analysis time, accumulation of rounding error and finally causes stiffness in the carbon structure. The results demonstrated that, the obtained elastic properties for the model with beam element were about 9% more than the three-dimensional model and also about 11% more than the continuous shell model. In addition, the elastic properties of the three-dimensional model are about 2% higher than the continuous shell model. It was also observed that for both armature and zigzag structures, shell, beam and three-dimensional elements give better results than each other, respectively. Understanding the results of this study helps to select the best type of element and arrangement for the analysis of carbon nanotubes in different conditions and applications. To check the accuracy of the results, the buckling behavior of carbon nanotubes with both zigzag and armature structures with beam, shell and three-dimensional elements under eccentricity has been performed. The results show that the selection of shell elements for carbon nanotubes with any structure gives better results and is in good agreement with the other reported results.

Introduction

Extensive research has been done on carbon nanotubes. The excellent properties of carbon nanotubes have led to their use as nanofibers in advanced reinforced composites. Reviewing previous research in this field, it can be clearly seen that the reason for the attraction to carbon nanotubes is their exceptional and remarkable properties. Due to the high cost of laboratory instruments, nanostructure modeling methods have found a special place in mechanical engineering to predict the behavior of materials at this scale.

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Nanoscale mechanical simulation methods enhance our ability to understand micro and nano-mechanisms in mechanical phenomena such as plasticity and failure [1-5]. Various experiments and theoretical researches have been used to describe the elastic behavior of carbon nanotubes, but there are always drawbacks to these analyzes [6-8]. Many researchers have focused their laboratory studies on the elastic properties of carbon nanotubes, but have usually reported a wide range of values for their mechanical properties. The reasons for this dispersion of the reported values can be seen in the use of various techniques in the experiment, the dissimilarity in the manufacturing methods and the lack of accurate direct measurement techniques at the nanometer scale or the problems that exist in the preparation of a test piece. One of the continuous environmental mechanics models presented here is the finite element model, which is adopted for modeling and analyzing the mechanical properties of carbon nanotubes [9-14].

In this research, the effect of element type and mesh size on changes in mechanical properties of carbon nanotubes has been investigated [15-18]. Selecting the appropriate element for the carbon structure of the nanotube and creating the desired network of elements has the greatest impact on the accuracy and convergence of the results. Due to the bonded and non-bonded interactions between carbon atoms, models such as truss model, space frame model and spring model have already been introduced [19-22].

The question is, because of the hypotheses and the type of elements used to simplify the models, can they accurately express the behavior of carbon nanotubes? Carbon is one of the most important elements in nature and its many applications in human life, well this point. Confirms [23-26]. Carbon is found in four different forms in nature, all of which are solid forms, and in these structures, carbon atoms are placed next to each other in a perfectly regular manner and can be bonded together and combined with other elements. Carbon atoms have an electron structure in terms of the order in which the orbitals fill, and have four free electrons that allow them to form four bonds [27-30].

These atoms form four unique covalent bonds in the diamond structure. That is, each carbon atom binds to four other carbon atoms. So, it has used all four of its capacities to form a link [31-33]. In the structure of graphite, nanotubes and fullerenes, there are also unique bonds between carbon atoms. The difference is that each atom only bonds to the other three atoms and therefore has three unique covalent bonds. In these structures, the carbon atom does not consume one of its capacities. This empty capacitance, which is actually an extra electron, forms a free bond outside the plane in which the other atoms are located [34-38].

This free or suspended bond can bond to other atoms in the environment under certain conditions. In nano-meter dimensions, there are several important parameters that have a great impact on the properties of materials [39-42].

History

Most popular and scientific papers attribute the discovery of hollow nanometer carbon tubes to Sumyajima from NEC in 1991. Carbon nanotubes may have been made even before that year, but it was not possible to observe these structures directly until TEM was invented. The discovery of carbon nanotubes by Ejima in the insoluble matter of graphene tubes burned in the soot resulting from the electric arc discharge of two carbon rods [43-46].

In a 2006 article in the Carbon Magazine, Mark Montiux and Vladimir Kuznetsov described an interesting, often distorted, origin of nanotubes [47-50]. Recently, carbon nanotubes have often been credited with the discovery of endothelium, and Ejima has been credited with clarifying the structure of nanotubes. One aspect of the structure of carbon nanotubes is their one-dimensional, empty interior structure. Their one-dimensional structure is of great interest to physicists because it allows them to experiment in one-dimensional quantum physics. Their empty structure is also of great interest to chemists because it allows molecules to be trapped, react in confined spaces, and release

molecules in a controlled manner for uses such as delivering drugs to the body [51-55].

In order to study carbon nanotubes by continuous environment methods, one of the most famous models created is the truss model, which was proposed by George Edgard and colleagues at the NASA Research Committee in 2002 to develop relationships between the structural properties of nanostructured materials [56-60].

Edgard's model was a volume element representing the chemical structure of graphene plate, which has been replaced by equivalent trusses and equivalent continuous models. A theory at the nanoscale of continuous environment was proposed by Zhang et al. [61], in which the continuous strain energy with the bond energy at the atomic level is calculated for all atomic bonds using Cauchy-Bourne law.

The theory was first used to study the elastic modulus of single-walled carbon nanotubes, then to study the fracture of the core of single-walled carbon nanotubes under tension. In various continuous medium findings, a representative volume element of the graphene chemical structure is replaced by an equivalent truss or other continuous medium models.

Lee and Chow [62] have replaced chemical bonding of atoms using a structural mechanical approach combining beam and molecular theory. They have shown that the mechanical behavior of an armature or zigzag carbon nanotube strongly depends on the diameter of the nanotube and slightly on its chirality.

Therps and Papanicus [63] proposed a three-dimensional finite element model for single-walled carbon nanotubes of armature, zigzag, and chiral, according to which the single-walled carbon nanotube under load would act as a beam-like structure. They concluded that the Young's modulus varies from TPa (1.06-0.6952) and the shear modulus to TPa (0.504-0.224) for a wall thickness of 0.34 nm [64-66].

Giannopoulos et al. [67] developed a discontinuous finite element method using a spring element to calculate the mechanical responses of single-walled carbon armatures and zigzags. In this model, instead of the beam elements proposed by Lee and Chow [68], linear elastic spring elements are used to model inter-atomic interactions.

In a new model proposed in 2008 by Marco Rossi et al. [69], a finite element model for determining the mechanical properties of single-walled carbon nanotubes, including the Young's modulus and ultimate stress and strain, was developed based on the theory of molecular mechanics. Nonlinear elements and torsional springs are used to model interatomic interactions.

The latest model of analytical molecular mechanics has been proposed by Chang and Yaw [70] in order to relate the elastic properties of a single-walled carbon nanotube to its atomic structure with the constant force field.

The analytical model of molecular mechanics developed by Zhao et al. [71] was developed under tensile and torsional loads to incorporate the Morse potential function to estimate the elastic constancy and to predict the stress-strain relationships for carbon nanotubes.

Wu et al. [72] also proposed an energy-equilibrium model based on the relationship between molecular mechanics and solid mechanics to study the mechanical properties of a single-walled carbon nanotube. In a recent model, Wu et al. Proposed an energy-equilibrium model for modeling single-walled carbon nanotubes. In this approach, they consider single-walled carbon nanotubes as a thin-walled cylinder under axial and torsional tensile loading. To model single-walled carbon nanotubes with an energy-equilibrium model, the author uses both the principles of molecular mechanics, and the potential energy of changes in the length and angle of the entire system. It is worth noting that in recent modeling, not only single-walled carbon nanotubes have been sufficient, but in their models, they have gone a step further and also model multi-walled carbon nanotubes [73-75].

Zhao et al. [76] have studied the deformation of single-walled and multi-walled nanotubes under internal pressure using an analytical molecular structural mechanic's model and considering the nonlinear interactions of van der Waals forces

between the layers. In their proposed model, Lee and Chow [77] considered each layer of multi-walled carbon nanotube exclusively as a wall with a frame-like structure, which used structural mechanical methods in their simulation. They also replaced the van der Waals forces between the layers with the Leonard-Jones potential and simulated them with nonlinear truss rod elements.

In another attempt, Kalamkarf et al. [78] developed a finite element model for modeling single-walled and multi-walled carbon nanotubes, which in an attempt to model the atomic interactions of covalent and van der Waals bonds with nonlinear beam and spring elements, respectively.

In the latest new model proposed in 2008 by Therps and Papanikos [79], which is proposed to model the elastic behavior of carbon nanotube-reinforced composites, a multidimensional representation volume element based on Morse's atomic potential is created [80].

The Investigation of Models developed to simulate the behavior of carbon nanotubes

The behavior and deformation of carbon nanotubes have been the subject of many experiments, molecular dynamics models, and continuous environment model studies. Experiments at this length scale are still in progress, so a range of values has been reported for various mechanical properties. Furthermore, compatibility in the interpretation of nanotube geometry remains an important issue when data are reduced to properties. Molecular dynamics simulations accurately show the structure of carbon nanotubes. Providing a suitable model that shows the behavior of carbon nanotubes with acceptable accuracy and also its use is economically justified is a very important factor. Based on the analysis of molecular dynamics and interactions between atoms, models are introduced [81-85].

These models, due to the assumptions made to simplify their use, are not able to fully cover the behavior of the carbon network in carbon nanotubes. Due to the excellent properties of carbon nanotubes, they are an important promise for use as nanofibers in advanced reinforced composites. Therefore, a thorough and accurate analysis of the macroscopic elastic properties of nanotubes is essential. Various experiments and many theoretical researches are used to describe the elastic behavior of carbon nanotubes. But there are always problems with these analyzes.

For example, many researchers have focused their laboratory research on the elastic properties of carbon nanotubes, but they usually report a wide range of values for mechanical properties. The reasons for this scattering of the reported values can be seen in the use of various techniques in the experiment, the dissimilarity in the manufacturing methods and the lack of accurate direct measurement techniques at the nanometer scale or the problems in preparing a test piece. In nanotubes, properties It is directly related to the geometrical parameters of the nanotube, which express the properties of the arrangement of atoms and the force field between them. The most classic form of continuous modeling of atomic systems is the theory of continuous environment or linear elasticity.

The advantage of this method is its ability to calculate the static and dynamic properties of the system. However, this simulation can affect the mechanical behavior of nanotubes by removing the atomic properties. Most activities in the continuous environment focus on the application of beam and elastic shell theories, and it is assumed that nanotubes remain coaxial during vibration or bending. As a result, their curvature can be expressed by a curve [86-89].

In continuous environment modeling, the effects of heat, quantum and electromagnetism are ignored. Due to the dependence of the nanotubes' response on their structure, a combination of scale analysis and continuous environment mechanics seems appropriate [6].

Simulation of Carbon Nanotubes

For simulation and numerical calculations, carbon nanotubes are replaced with an equivalent structural model. The interrelationships between molecular mechanics and structural mechanics are used to

balance the two models. The structural model is then analyzed using the finite element method. Finally, the model undergoes pure stretching and twisting. The net tensile simulation is performed by binding both degrees of transverse and rotational freedom at one end of the nanotube, while the nanotube is loaded with tensile loads at the other end. Similarly, the net torsion conditions on the carbon nanotubes are fully bound at one end of the radial motion (UR = 0).

Modeling of carbon nanotubes with beam elements Since carbon atoms in both rolled graphene sheets and nanotubes are bonded together by covalent bonds of specified bond length, carbon atoms can be seen as material points bonded together by load-bearing elements. The modeling is based on the assumption that carbon nanotubes act as a space frame when loaded. The bond between carbon atoms is considered as load-bearing members, while atoms act as joints for members. they do. In this model, the nodes are placed in the position of carbon atoms and the carbon bonds between them are modeled using elastic beam elements (Fig. 1).

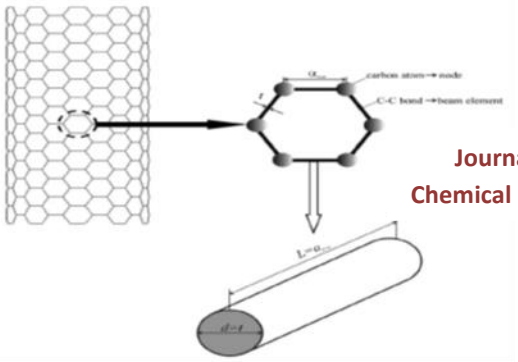

Figure 1. Simulation of carbon nanotubes as a space frame [1]

In the molecular stage, the interaction between carbon atoms is described using the force field associated with the nucleus-nucleus interaction and the nucleus-electron interaction [90].

Excluding electrostatic relations, the total potential energy (Utotal) that characterizes the force field is obtained by summing the energies of the bonded and non-bonded interactions [73].

$$U_{total} = \sum U_r + \sum U_\theta + \sum U_\varphi + \sum U_{vdw}$$

Here Uvdw Ur, Uθ, Uφ refer to the energies associated with bond tension, bond bending, bond torsion (in-plane and off-plane), and forces and undervals (non-covalent), respectively. Figure 2 shows the types of interactions atomic in the molecular stage. The potential energies for covalent bonds between carbon atoms are defined by the following equations.

$$U_r = \frac{1}{2}k_r(r - r_0)^2 = \frac{1}{2}k_r(\Delta r)^2$$

$$U_\theta = \frac{1}{2}k_\theta(\theta - \theta_0)^2 = \frac{1}{2}k_\theta(\Delta\theta)^2$$

$$U_\varphi = \frac{1}{2}k_\varphi(\Delta\varphi)^2$$

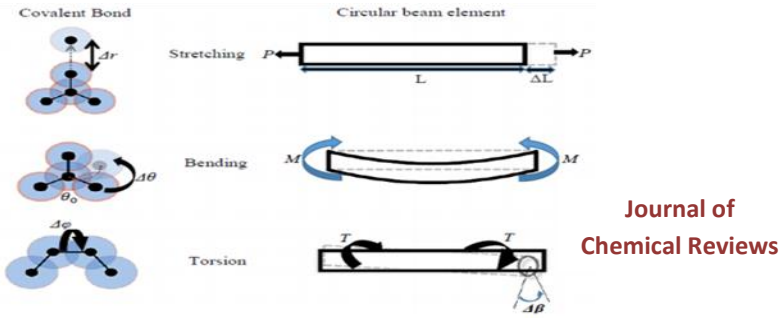

Figure 2. Equilibrium of molecular mechanics and structural mechanics for covalent and non-covalent interactions between carbon atoms [4]

Here, r0 θ0 refers to the atomic distance of a bond in the free state and the angle of the bond in the free state (as shown in Figure 2), and the values of r and θ refer to the distance and angle of the bond after deformation. . As a result, the parameters Δθ, Δr and Δφ indicate changes in bond length, bond angle and torsional angle of the bond, respectively.

The parameters kφ kθ, kr represent the force constants related to the tension, bending and torsion of the chemical bond. Carbon atoms in nanotubes with covalent bonds with a specific bond length and a specific bond angle hold their position together and bind any displacement of carbon atoms against molecular forces [44]. Non-bonding interactions such as van der Waals forces are well described using the Leonard-Jones potential. This potential was proposed by John Lenard-Jones in 1924 [90-92].

The Lenard-Jones potential is an approximate potential for describing the interaction between two particles (atoms or molecules), which have gravitational forces at long distances and repulsive forces at close distances. The abduction force is usually the van der Waals force and the driving force is the thrust force due to the overlap of the two-part electron cloud. This potential is an approximation and has not been derived from a more fundamental theory. The energy associated with the van der Waals bonds is expressed by the Leonard-Jones potential as relation.

$$V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

In Equation above, the parameter σ denotes the distance at which the potential becomes zero in terms of nm and ε denotes the depth of the potential well in terms of kJ/mol, and the parameter r denotes the distance between the related particles. These are a property of the material and are determined by the nature and strength of the bond. These parameters are usually determined by fitting laboratory data or by accurate calculations in quantum chemistry [2].

The factor that causes the change of Young's modulus values in the tables and diagrams above is the type of element and the mesh density. This increase in the number of elements results in a range of elements. Relate to each of the structures to converge with the three-dimensional beam and shell elements. It is also observed that the modulus of elasticity of the zigzag structure is always less than the corresponding value of the armature arrangement and ultimately it is not possible to exceed the values of the armature structure. What has been found in all of these models is that the results of the answers are closer to the results reported in other studies as the mesh becomes smaller and the number of elements increases.

The Young's modulus obtained from the beam element is closer (about 1% less) than other results with the same type of element. In this regard, the Yang modulus obtained with shell elements (about 1.84% less) and then the three-dimensional elements (with 12.67% less) with the reported Yang modulus, respectively, other studies with similar elements differ. In table 1 The effect of nanotube thickness on the Young's modulus of single-walled carbon nanotubes is shown. It can be seen that the thicker it is, the smaller the Young's modulus obtained.

Table 1. Young modulus reported for different thicknesses of armature carbon nanotubes (8,8) and zigzag (0,14)

(0‹14) E(TPa)	(8‹8) E(TPa)	Wall thickness t (nm)	Method	researchers
5.728	5.269	0.066	Molecular dynamics	Jacobsen et al.
4.705	4.721	0.074	Tight Binding Model	Zhou et al.
4.664	4.634	0.075	Approximate model of local density	Lee et al.
2.5990	2.6062	0.144	limited parts	Sobhan Safarian
2.5683	2.5752	0.145	limited parts	Sobhan Safarian
2.3915	2.3976	0.1466	limited parts	Sobhan Safarian

Conclusion and Recommendations

Carbon has a direct effect on all aspects of our lives. We are made of carbon, we eat carbon, and our civilization, our economy, our homes, and the basis of our daily transportation are all built on carbon. We need carbon, and without it, the very foundations of daily life we know will fall apart, but this coin has another side that is known today as global warming. Carbon is now the number one culprit in global warming. Carbon is highly regarded for its important role in the bonding of stem molecules in our lives and for the unique nature of the carbon-carbon bond.

It can be said that it has more applications than any other nanostructure. The mechanical properties and amazing behavior of carbon nanotubes are increasingly attracting the mechanical engineering community. In this research study, the behavior and properties of carbon nanotubes were investigated and the models developed by SOLIDWORKS Similation software were examined. The results are summarized as follows:

- It was observed that the mechanical properties of carbon nanotubes are strongly dependent on the wall thickness. The Young's modulus for both armature and zigzag single-walled nanotubes increases with increasing diameter, which is due to the increase in the principal parameter n (increasing length) of the chiral nanotube vector. Armchair specimens have a higher modulus of elasticity and shear modulus.
- The yang modulus obtained in traction for the model with the beam element is about 4.2% higher than the three-dimensional model and also about 4.9% higher than the continuous shell model. Also, the elastic properties of the 3D model are about 9.3% higher than the continuous shell model.
- The average Yang modulus obtained in traction for a model with a beam element is about 1% less than the value reported with the same type of element.
- The average Young modulus obtained for a model with a three-dimensional element is about 12.67 less than the value reported with the same type of element.
- The calculated Young's modulus for a model with a shell element is about 1.84% lower than the reported value of a model with the same type of element. The shear modulus obtained by tensile test for the model with the beam element is about 3.3% higher than the three-dimensional model and also about 1.9% higher than the continuous

shell model. The shear modulus obtained from the tensile test of a model with a three-dimensional element is about 1.4% higher than that of a continuous shell model. The shear modulus obtained by torsion testing for the model with the beam element is about 3.7% higher than the three-dimensional model and about 7% higher than the continuous shell model. Also, the shear modulus obtained from the tensile test of the model with a three-dimensional element is about 3.1% higher than the continuous shell model.

- The obtained shear modulus for the model with the beam element is about 1.9% less than the value reported with the same type of element.
- The Young's modulus obtained for a model with a three-dimensional element is about 10.48% lower than the value reported with the same type of element.
- The calculated yang modulus for the model with the shell element is about 4.4% less than the reported value of the model with the same type of element. The Young's calculated modulus for this study is about 5.17 % lower than the results reported by other studies.
- The calculated shear modulus of this research is about 5% less than the results of other researches. Poisson's ratio of this study is about 2% lower than the results of other studies.
- Carbon nanotubes modeled with shell, beam and three-dimensional elements provide good results, which are evident in the results obtained for the buckling of carbon nanotubes with different structures.

Nanotubes retain their round cross-section in buckling, and their deformation occurs entirely from the side, very similar to beam bending. Buckling In some nanotubes, local and semicircular buckling occurs along the tube, but its axis, like shell buckling, remains straight. The results of this study are consistent with what has been said in the references. The modeling results presented in this study also confirm the axial properties of previously obtained single-walled carbon nanotubes. A very good agreement was observed between the results calculated in this study and the given results, and this agreement also shows the ability of the developed models to provide an accurate picture of the behavior of single-walled carbon nanotubes. Finally, it should be noted that in the models obtained from some theoretical and laboratory methods, due to the difficulty and problems of loading and measuring data at the nanoscale, the mechanical properties of carbon nanotubes cannot be fully and accurately calculated, and this is more comprehensive methods. The modeling and analysis of carbon nanotubes used in this research.

Recommendation

According to the modeling and analysis of carbon nanotubes, the above models can be used to determine the deformation and radial stiffness. As mentioned, in modeling carbon nanotubes, the effect of the type and number of elements can be applied to multi-walled nanotubes to better understand the properties of this amazing material. These suggestions can be used as future activities in order to achieve a more complete and better understanding of the behavior of this nanostructured material uniquely or in interaction with other materials. It can be said that the use of models with continuous shell elements for research study of multilayer carbon nanotubes under different loads (due to the relatively complex structure and the need for very high calculations) is a desirable choice.

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