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Original Research Article

Probabilistic mechanical properties and reliability of carbon nanotubes

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ABSTRACT

Carbon nanotubes (CNTs) and their products such as polymer nanocomposite (PNC) are an undeniable part of future materials. To use such future materials, it is necessary to have an accurate evaluation of their properties. Several uncertainties such as structural defects and their distributions cause change in the properties of CNTs that could be considered probabilistic variables. A novel procedure is presented for evaluating CNTs' probabilistic fracture properties and structural reliability using stochastic finite element methods. By employing two dimensionless parameters, both types of Stone–Wales 5-7-7-5 defects are randomly applied to CNTs. Section defect density and critical section defect density are defined and used to manage the distribution and geometrical configuration of CNTs' structural defects. A probabilistic method is used to evaluate the effect of defects' distribution on Young's modulus, ultimate strain, and ultimate stress. It has been observed that normal and Weibull distribution functions are suitable for describing Young's modulus distribution and ultimate stress distribution, respectively. Defect density ratio is defined and, using this parameter, the effect of aggregated defects on mechanical properties is evaluated. It is demonstrated that the defects out of critical section have an unavoidable effect on Young's modulus and ultimate strain; but they have an insignificant effect on ultimate stress. A reliability analysis is performed on armchair (15,15) CNTs and it is investigated that the reliability of CNTs depends on critical defect density significantly. In addition, the reliability is equal to one for the stress of less than 50 GPa and this value is equal to zero for the stress of higher than 100 GPa, independent from the changes of critical defect density. Eventually, a procedure is described to estimate the reliability of armchair CNTs using critical defect density and the results' accuracy is discussed and evaluated.

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1. Introduction

There is no doubt about the fact that CNTs have been considered new generation materials. Accordingly, CNTs receive a great deal of attention, since their discovery by Iijima in 1991 [1]. This huge amount of attention has been related to CNTs' extraordinary properties. They present exceptional properties such as small size, low density, high stiffness, high strength, high electronic conductivity, and

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perfect thermal properties [2,3]. Although many synthetic methods have been developed for the controlled design of CNTs, there is evidence that defects can appear during device and composite production or under mechanical strains [4].

Decreased mechanical properties, due to even a small number of defects in atom structures, have been indicated in previous works [5,6]. Studies have shown that defects significantly influence not only mechanical properties but also other important properties such as chemical and electrical properties [7,8].

Moreover, to achieve the desired functionality, defects in CNTs can be created by chemical treatment or irradiation [9,10]. For example, defects increase the interaction between CNTs and polymer matrix in PNC, which provides more improved properties [11].

Furthermore, some researchers believe that defects could have an improvement effect on the overall characteristic of bundles of single-wall carbon nanotubes (SWCNTs) and multi-wall carbon nanotubes (MWCNTs). They believe that, using some chemical methods such as irradiation, it is possible to create defect-mediated covalent bonds between SWCNT in bundle [26–28] or between shells of MWCNT [29,30]; however, in defect-free SWCNT bundles or MWCNT, the interaction between CNTs are constructed by weak Van der Waals forces. Experimental studies on electron irradiation and mechanical testing on bundle of CNTs have introduced that small dose irradiation gives rise to notable enhancement in the mechanical properties of the irradiated one. It should be considered that high dose of irradiation has improvement effects on shear module inside the bundle. On the other hand, high dose of irradiation causes damage to the atomic network of CNTs.

Moreover, coalescence and welding of CNTs are critical requirements in several sciences such as engineering of nano-circuits. Irradiation demonstrates ways to linking nanotubes by covalent bonds. However, even spatially-localized irradiation creates defects not only in the junction region, but also in the rest of the system such as sputtered carbon atoms. Therefore, to study the effect of defects in mechanical properties, the most important uncertainties in this research are the CNTs' structural defects and their distribution.

The CNTs and their structural defects have been modeled by various numbers of methods. In this research, choosing an appropriate method for modeling is a challenge between the accuracy of result and computational cost of solving process. For instance, the approaches based on quantum, including ab initio, molecular dynamics (MD), and density functional theory (DFT), are much more computationally expensive, but present accurate results [12,13]. These methods are suitable for demonstrating physical phenomenon and analyzing small group of atoms. For modeling an issue in industrial applications, atomic-based method has several limitations such as dimension and time in nanometer and picosecond, respectively. Due to the mentioned difficulties in quantum simulation, choosing another simulation method for modeling CNTs' structure and evaluation of different uncertainties is more applicable.

There are also some continuum-based methods such as continuum structure mechanics model [14], continuum truss methods [15], and analytical molecular mechanics methods [16–18]. By these methods, modeling of bond breaking process is not naturally possible. In order to use this method for modeling the fracture of bonds, modifications by changing the potential function and introducing nonlinear finite element methods are essential. The selection of appropriate inter-atomic potential function is an important requirement for modeling the bond breaking process. For example, by employing harmonic energy potential function, the researcher can have accurate results only for elastic constant parameters such as Young's modulus and Poisson's ratio near the equilibrium position. The more accurate and versatile one is called Brenner potential function. Continuum mechanic approaches that have used Brenner potential function have studied elastic properties and stress–strain relationship based on modified Cauchy–Born rule [19]. According to the increased number of models in this approach, computationally expensive methods such as MD, ab initio, and quantum methods may have unconstructive effects on research process.

Another inter-atomic potential function which is appropriate for bond breaking model is called Morse potential function [20]. This potential function has been used by many researchers for modeling both CNTs with and without defect under different type of loads [14,21]. Researchers are able to predict the nonlinear stress–strain relationship including CNTs' atomic structure ultimate stress and ultimate strain. In this approach, the analytical model is developed to evaluate mechanical response of both SWCNT and MWCNTs under internal and external pressures.

Moreover, in mass production, each nanotube has individual structural properties [22,23] which are influenced by parameters such as size, chiral indices, various types of defect, etc. Because the individual analysis of properties of all CNTs is impossible, an alternative stochastic method could be used to demonstrate the properties in terms of probability distribution of CNTs' structural uncertainties. Using this approach, researchers can evaluate probabilistic properties of an applicable system by modeling several species. The probabilistic properties of fiber composite and PNC materials have been published in different reports [24–29]; but, there is no information about the probabilistic mechanical properties of CNTs.

2. An atomistic based nonlinear finite elements method

SWCNT is demonstrated as rolled graphene sheet. By this method, the configuration of SWCNT structure is defined as a direction of rotation, which is represented by a pair of indices that are both integer numbers. They denote the number of unit vectors along two directions in the honeycomb crystal lattice of graphene [30]. When n and m are equal, CNTs are called armchair; when m is equal to zero, CNTs are known as zigzag. Otherwise, they are called chiral. The diameter of an ideal carbon nanotube in pm can be calculated as follows [31]:

$$d = \frac{a}{\pi}\sqrt{n^2 + nm + m^2} = 78.3\sqrt{(n+m)^2 - nm} \tag{1}$$

where $a = 0.246$.

According to MD investigations, overall empirical inter-atomic potential energy of a molecular system is demonstrated

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