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EFFECT OF CNT LENGTH AND INTERFACE WAVINESS ON EFFECTIVE MATERIAL CONSTANT (E_z) OF CNT-BASED COMPOSITE MATERIAL

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ABSTRACT

High performance composites are currently being used in the marine, automotive, aerospace and defense industries. These industries demand materials with properties that are similar or better than conventional metals at fraction of the weight. Among different properties of materials required for designing products, effective material constant (E_z) is important one. In this paper, two parameters, carbon nano tube (CNT) length and wavy interface are considered for calculating E_z of a CNT based composite material using finite element analysis method. In first case, E_z has been determined with various CNT lengths in a representative volume element (RVE). It shows that E_z increases linearly with the increase of CNT length. Again, E_z is determined for wavy interface in a RVE with various cycle numbers. In this case, E_z increases slightly with the increase of cycle number in the wavy interface between CNT and matrix.

Keywords: Carbon Nanotube Reinforced Polymer, FEM-Finite Element Method

1. INTRODUCTION

Although many definitions of 'composites' are available, they can be described as materials comprised of two or more constituents with very distinct compositions, structures and properties separated by an interface. The aim in producing composites is to combine different materials in a single device with properties that cannot be obtained from the individual components. Therefore composites for optical, structural, electrical, opto-electronic, chemical and other applications are easily found in modern devices and systems. During the past 30 years, there has been a substantial development of composites for structural applications. The main support of this tendency is the possibility of producing composites with high mechanical properties and low density that can replace traditional materials such as steel and wood. The combination of high performance polymers with high modulus-high strength ceramic or polymer fibers allowed the production of composites with a group of properties per weight superior than those of steel, aluminum and others [1].

In the technologically advanced era that we currently live in, there is a growing demand for cheaper and more durable materials for a variety of applications. Previously metals and metals alloys were used to manufacture anything and everything from paper clips to skyscrapers. Then plastics were discovered and a revolution began where plastics started replacing metal components, for example, gears, bearings, etc. plastics are easier to mould into complex parts as well as being lighter than their metal counterparts and just as durable. Initially plastics were expensive, but as their application and demand in everyday life increased, the manufacturing costs of plastic components decreased.

The use of plastic components are limited to low end application such as food containers and dustbins due to their relatively low strength. High end applications such as automotives, marine and aerospace structures still required the use of metals and their alloys. Thus, strong but lightweight materials and composites are needed to be developed.

Reinforcement of carbon nanotube has been employed successfully for over many years as means of improving the mechanical properties of the manufactured products. Combining high-modulus, high-strength carbon nanotube with a polymeric matrix produces a composite material with higher stiffness and strength, and lower thermal-expansion coefficient. The reinforcing nanotubes can be introduced either in continuous (long) or discontinuous (short) form. While continuous nanotube provides greater improvement of the mechanical properties, they also significantly complicate composite-material processing. Short-nanotube composites, on the other hand, can be easily manufactured by automated and hence more economical methods [2].

1.1 Objectives

The objectives of this research is to analyze the effect of Carbon nanotube length (CNT) and interface waviness on effective material constant (Ez) of carbone nanotube-based composite material using finite element analysis method (FEM).

2. LITERATURE REVIEW

It is an interesting fact that many natural forms of reinforcement possess a nanometric dimension, whereas most current synthetic composites include fibers in the micrometer range. Expected benefits of such “miniaturization” would range from a higher intrinsic strength of the reinforcing phase (and thus of the composite) to more efficient stress transfer, to possible new and more flexible ways of designing the mechanical properties of yet even more advanced composites. First these arguments are reviewed, and then the concept of stress transfer leading to the principle of reinforcement is discussed. This is followed by specific materials aspects and by a short account of possible future forms of reinforcement [3].

Another important feature of composites is that they can also be easily designed to fit in a specific application due to the capability of having their properties tailored by changing one of a series of variables. Some of these variables are the type, concentration, size, shape and orientation of the constituents. Among these variables, the shape and the orientation of the reinforcing agent are the components of recognized importance in the design of composites. The influence of the aspect ratio of short fibers on the properties of composites is well documented and dictates the overall stress transferability phenomenon. Free fiber ends do not contribute to stress transfer. Stress is built progressively from the fiber ends up to a certain length (fiber critical size) where the stress transferred to the fibers reaches the characteristic maximum value for a specific system [1].

Structural composites are engineering materials made of oriented reinforcing fibers dispersed in a metallic, ceramic or polymer matrix. The use of composites moved forward in components of aircrafts and space structures mainly due to project flexibility, easy processing, lower density (0~2 g/cm^3), as well as high mechanical strength and modulus, that match the requirements of the structures during service [4, 5]. This turns the composites particularly attractive as substitutes of the metallic alloys for high demanding aeronautical and space applications [4].

The behavior of the fiber (CNT)-reinforced composite materials has been experimentally studied in many aspects mostly under tensile and compressive load by the Split Hopkinson Pressure Bar (SHPB) method, as it gives the properties of the test materials over a wide range of strain rates [6, 7].

In impact to determine the mechanical properties of composite materials under dynamic tensile loads, a review of technique was given by Harding and Welsh [8]. In the standard tensile version of folksy bar apparatus the input loading bar become the weigh bar tube within which the output bar slides freely. Dynamic stress strain curves for unidirectional reinforced carbon epoxy composite in which failure occurs in less than 30μs at a mean strain rate of about 400s^{-1} and for woven reinforced glass/epoxy composites with the time to failure approach 100μs and average strain rate was around 1000s^{-1} were presented and their validity was established by the authors.

Toward this objective, Pardon and Batiste [9] performed tension tests of unidirectional e-glass/polyester composite specimens on a Scheck high strain rate hydraulic test machine to investigate the effect of strain rate on the tensile strength of material.

Hayes and Adams [10] conducted various tests at various tests speeds and load levels to characterize the tensile impact behavior and rate sensitive materials properties of unidirectional glass/epoxy and CNT/epoxy composites.

Peterson and pentane [11] tested five different materials and ultimate strength; failure strains and effective module for each material were investigated as function of strain rate under dry and wet test conditions. The authors got a different type of results here in terms of failure strains for the materials tested.

Liu and Chen evaluate the effective material properties of carbon annotate-based composites using a nonsocial representative volume element (RVE) [12]. Hayes et al. determined Fiber/Matrix stress transfer through a discrete interface or interphone [13]. Linier Zhu and Kwabena A Narh evaluate the effect of nanotube orientation on tensile modulus of carbon-nanotube-reinforced polymer composites [14]. Liaoa and Li reported a study on the interfacial characteristics of a carbon nanotube (CNT)-reinforced polystyrene (PS) composite system through molecular mechanics simulations and elasticity calculations [15].

Khare, R. et al. and Harris [16, 17] reviewed few recent researches on carbon nanotube composites. The interfacial bonding properties, mechanical performance, electrical percolation of nanotube, polymer and ceramic are also reviewed. On the other hand, Shin et al. examined electrical conductive composites [18] and Nan et al. [19] examined electrical conductive composites based on carbon nanotube. Very recently Unnati et al. [20] evaluated the effective material properties of CNT-based composites using a square representative volume element (RVE) based on the continuum mechanics and with the finite element method (FEM).

3. METHODOLOGY

In this research the effect of Carbon nanotube length (CNT) and interface waviness on effective material constant (E_z) of carbone nanotube-based composite material is analyzed using finite element analysis method (FEM). E_z is determined by FEM using software Ansys_10 and from the Eq. (1), (2) and (3). In this case, the RVE can be divided into two segments: one segment accounting for the two ends with total length L_e and Young’s modulus E^m; and another segment accounting for the center part with length L_c and the effective Young’s modulus E^c. Note that the two hemispherical end caps of the CNT have been ignored in this derivation.

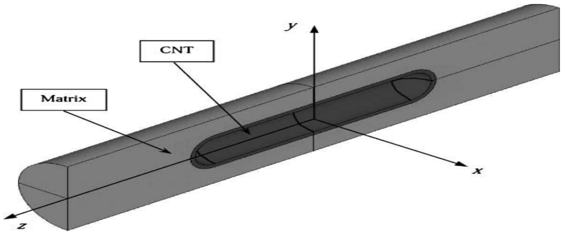

Fig 1. Cylindrical RVE containing a short CNT shown in a cut-through view.

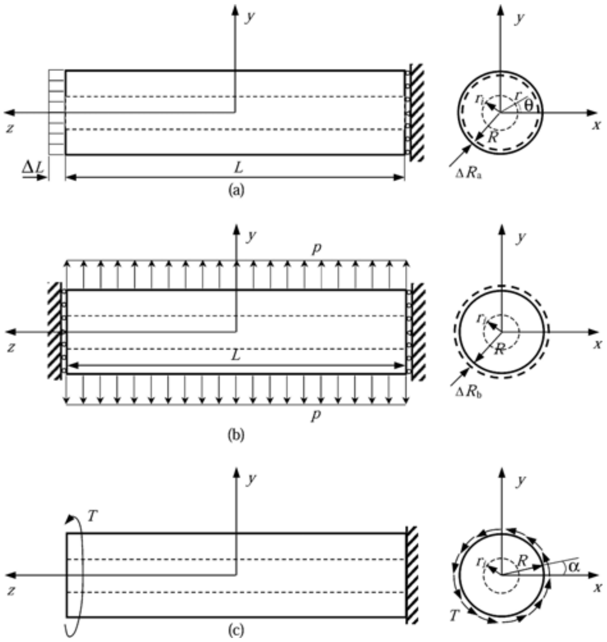

Fig 2. The cylindrical RVE used to evaluate the effective material properties of the CNT-based composites: (a) under axial stretch ΔL; (b) under lateral uniform load P; (c) under torsional load T.

For the center part the effective Young's modulus is found by-

$$E^c = E^t V^t + E^m (1 - V^t) \qquad (1)$$

Here, V^t is the volume fraction of CNT and is given by-

$$V^t = \frac{\pi(r_0^2 - r_i^2)}{\pi(R^2 - r_i^2)} = \frac{(r_0^2 - r_i^2)}{(R^2 - r_i^2)} \qquad (2)$$

Again, by considering the compatibility of strains and equilibrium of stresses, one obtains the following expression for the effective Young's modulus in the axial direction:

$$E_z = \left[\frac{1}{E^m}\left(\frac{L_e}{L}\right) + \frac{1}{E^c}\left(\frac{L_c}{L}\right)\left(\frac{A}{A_c}\right) \right]^{-1} \qquad (3)$$

Here, $A = \pi R^2$ and $A_c = \pi (R^2 - r_i^2)$.

4. RESULTS AND DISCUSSION

As described earlier, the study has been conducted for two cases: changing length of CNT in RVE and changing cycle number for wavy interface in RVE between CNT and Matrix. Both cases have been illustrated below.

4.1 Results for Varying Length of CNT

Simulations are done for different length of CNT in RVE. For all model, all properties for matrix and CNT remain constant, only CNT length varies in a range from 20nm to 80nm in a 100nm long matrix. For each length of CNT E_z is determined from Eq. (1), (2) and (3) and from FEM. Then both results are compared.

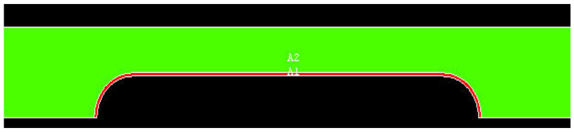

Fig 3. A cylindrical RVE for a short CNT in a matrix (CNT length=60nm and matrix length=100nm).

4.1.1 Results From Direct Equation

Figure (4) shows the graphical representation of how effective material constant (E_z) varies with CNT length (using Eqs. (1), (2) and (3)). From graph it is clear that effective material constant (E_z) increases linearly with the increase of CNT length. The relationship between E_z and length of CNT (L) is as Eq. (4), where correlation coefficient R=1. As the slope of the regression equation (4) is positive, increasing trend is evident.

$$E_z = 0.063\,L + 199.9 \qquad (4)$$

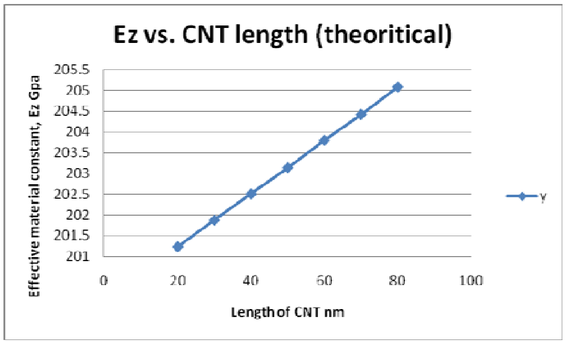

Fig 4. E_z (theoretical) versus CNT length Curve

4.1.2 Results from FEM

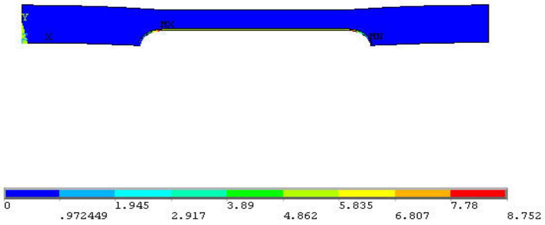

Fig 5. Plot of the first principal stresses for the short CNT model under the axial stretch, ΔL = 1nm.

Using FEM effective material constant E_z is determined for different CNT length. Figure (6) shows how E_z (from FME) varies with CNT length. From graph we can see that E_z increases with the increase of CNT length. But the increasing pattern is not linear as previous. The relationship between length of CNT (L) and E_z calculated from FEM can be expressed as Eq. (5), where correlation coefficient R=0.9864. As the slope of the regression equation (5) is positive, increasing trend is evident.

$$E_z = 0.149L + 198.5 \qquad (5)$$

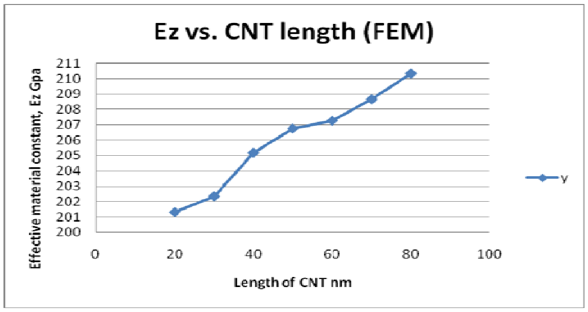

Fig 6. E_z (FEM) versus CNT length Curve

4.2 Simulation Results for Varying Cycle Number in Wavy Interface

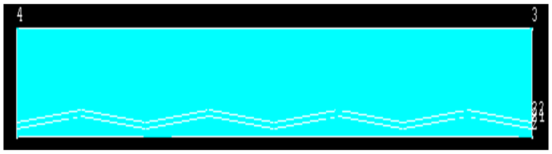

Fig 7. A RVE wavy interface between CNT and Matrix containing cycle number 2

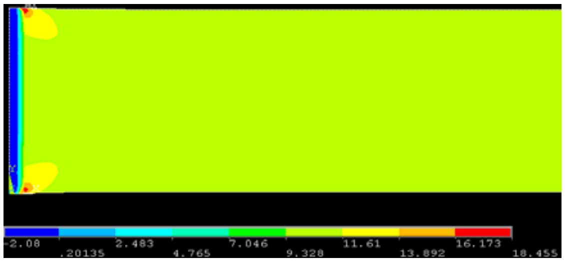

Fig 8. Plot of the 1st principal stresses for the short CNT model under the axial stretch, ΔL = 1nm.

In this case simulations are done for different cycle number in wavy interface between CNT and matrix. In figure (9) the computed effective material constant (E_z) for different cycle number in wavy interface is plotted against cycle number. From graph it is clear that E_z increases slightly with the increase of cycle number in wavy interface between CNT and matrix. From cycle number 0 to 3 the graph shows that the increasing trend is not fully linear. This fact can be explained by correlating E_z and cycle number (C_n) in wavy interface. A 4th order polynomial equation (Eq. 6) can be best suited for correlating E_z and C_n with correlation coefficient R=1.

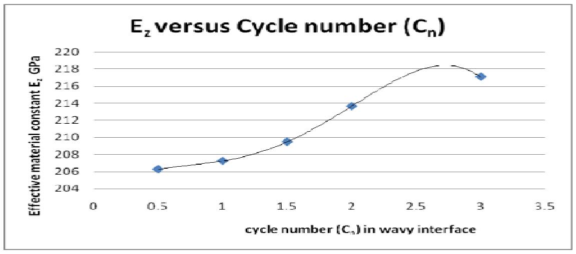

Fig 9. E_z (FEM) versus Cycle number in wavy interface

$$E_z = -1.773C_n^4 + 9.747C_n^3 - 15.61C_n^2 + 11.62C_n + 203.2 \quad (6)$$

The effective mechanical properties of carbon nanotube-based composites are evaluated using a 3-D nanoscale RVE based on 3-D elasticity theory and solved by the finite element method. Formulas to extract the material constants from solutions for the RVE under three loading cases are established using the elasticity. An extended rule of mixtures, which can be used to estimate the Young's modulus in the axial direction of the RVE and to validate the numerical solutions for short CNTs, is also derived using the strength of materials theory. Numerical examples using the FEM to evaluate the effective material constants of a CNT-based composites are presented, which demonstrate that the reinforcing capabilities of the CNTs in a matrix are significant. With only about 10nm increasers of the CNTs in a matrix, the stiffness of the composite in the CNT axial direction can increase in a range between 0.5% to 1.4percent for the case of short CNT fibers. And the effective material constant (E_z) also increases with the increase of cycle number in a wavy interface of CNT-based composite material between CNT epoxy matrix.

Many research issues need to be addressed in the modeling and simulations of CNTs in a matrix material for the development of nanocomposites. Analytical methods and simulation models to extract the mechanical properties of the CNT-based nanocomposites need to be further developed and verified with experimental results. The analytical method and simulation approach developed in this paper are only a preliminary study. Different type of RVEs, load cases and different solution methods should be investigated. Different interface conditions, other than perfect bonding, need to be investigated using different models to more accurately account for the interactions of the CNTs in a matrix material at the nanoscale. Nanoscale interface cracks can be analyzed using simulations to investigate the failure mechanism in nanomaterial.

5. CONCLUSION

In the technological era, the importance of composite material is infinity. But it is difficult to make a composite material with proper characteristics, because a number of parameters affect the composite's strength, such as fiber length, interface thickness, wavy interface, volume fraction of fiber, volume fraction of matrix, and so on. Many researches show that CNT-based composites are better than others.

Many researches have been carried out and many researches are running on composite material. But their objective is almost same how to improve their properties? In this paper two parameters are considered CNT length and wavy interface. E_z was determined with various CNT lengths in a RVE. This work shows that effective material constant increases almost linearly with increase of CNT length. Again E_z was determined for wavy interface. This part of study was carried out with various cycle numbers in wavy interface in a RVE. The result showed that effective material constant increases slightly with the increase of cycle number in the wavy interface between CNT and matrix. With only about 10nm increasers of the CNTs length in a matrix, the stiffness of the composite in the CNT axial direction can increase in a range between 0.5% to 1.4percent for the case of short CNT fibers.

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7. NOMENCLATURE

Symbol	Meaning	Unit
RVE	Representative Volume Element	
CNT	Carbon Nano Tube	
FEM	Finite Element Method	
E_z	Effective Material Constant	GPa