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SOLID MECHANICS

NEW THEORY TO PREDICT THE ELASTIC MODULUS OF CARBON NANOTUBE BASED-COMPOSITES

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ABSTRACT: The relatively weak mechanical properties of polymer have prevented its application in the components which demand high mechanical strength and stability. There are numerous theories with special assumption on the mechanics of nanocomposite to predict the elastic modulus. However, some of these theories can be efficient to consider the influences of CNTs on elastic properties of nanocomposite reinforced CNTs. Current research focuses on creation a new model base on new assumption with just having single fiber to predict the elastic modulus of nanocomposite reinforced CNTs. To verify the predictions of the new model we used experimental data and some well-known theories. Errors at most of the models were more than 10%, while by using this new model, errors has been decreased.

KEY WORDS: Carbon Nanotubes, Mechanical Properties of Nanocomposites, Polymer Matrix Composites, Elastic Modulus, Nanocomposite Modeling.

1 INTRODUCTION

Nanocomposite is a mixture of two distinct constituents, reinforcement and matrix, with remarkably different properties [1–4]. Recently, nanoparticles have been attracting increasing attention in the composite community because they are capable of improving the mechanical and physical properties of traditional fiber reinforced composites [5–9]. CNTs have many structures, Multi-walled carbon nanotubes (MWNTs) and single-walled carbon nanotubes (SWNTs) which are the most well-known type of CNTs. In 1991, MWNTs consist of many coaxial graphite cylindrical tubes and in 1993; Sumio Iijima discovered SWNTs with one graphite cylindrical tube [10]. MWCNTs and SWCNTs were discovered in soot of arc-discharge method and using metal catalysts in arc-discharge method [11,12]. Polymer matrixes generally combine high-strength, high-stiffness fibers (CNT, kevlar, etc.) with low-density matrix materials (epoxy, polyvinyl, etc.). The relatively weak mechanical properties of polymer have prevented its application in CNTs with the outstanding elastic modulus of 1 TPa, tensile strength of 63 GPa and high aspect ratio are among

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the strongest and stiffest reinforcements. The notable mechanical properties make CNTs to become one of the most intensively studied materials and ideal choice as reinforcement in metal, polymer and ceramic matrix nanocomposites [13–16].

There have been numerous theories and well-known models with special assumption on the mechanics of nanocomposite to predict the elastic modulus such as (Halpin-Tsai equation, shear lag, etc.). Halpin and Tsai were presented an equation that is efficient to predict the modulus values for the fiber reinforced composite samples; now Halpin-Tsai equation is used to predict the elastic modulus of nanocomposite reinforced CNTs [17–19].

Researchers have modified the Halpin-Tsai equation. Cox proposed an orientation factor parameter to account the randomness of discontinuous fibers [20]. Meng et al. used the orientation factor to obtain the effective elastic modulus of CNTs to modify the Halpin–Tsai equation [21]. At the nanoscale, the structure of the carbon nanotube strongly effects on the properties of composite. Thostenson and Chou developed a fundamental understanding effect of the CNTs structure on the elastic properties of nanotube-based composites. They used Halpin-Tsai equation through modifying the micromechanical approach to model short fibre composites to the account for the structure of the nanotube reinforcement to predict the elastic modulus of the nanocomposite as a function of the constituent properties, reinforcement geometry and nanotube structure. Their result shown that nanocomposite elastic properties are particularly sensitive to the nanotube diameter, since larger diameter nanotubes show a lower effective modulus and occupy a greater volume fraction in the composite related to smaller-diameter nanotubes [22]. And base on filler, there is further modification of the Halpin-Tsai equation by using different shape factor [21–23].

Shear lag theory have been used to consider the effect of the aspect ratio on elastic properties of nanocomposites reinforced CNTs [24]. In considering the elastic properties of nanocomposite reinforced CNTs, other theories give result with high error.

Current research focuses on creating a new model base on new assumption with just having single fiber to predict the elastic modulus of nanocomposite reinforced CNTs. The correlation of the experimentally obtained elastic modulus showed a good agreement with this model.

2 METHODOLOGY

2.1 HALPIN-TSAI MODEL

The Halpin-Tsai equation has been recognized for its ability to predict the modulus values for the fiber reinforced composite samples. This equation was used to correlate the experimental findings. For convenience, the equations are shown below [17, 18]:

$$E_c = E_m\left(\frac{1+(2l/d)\eta v_f}{1-\eta v_f}\right), \tag{1}$$

$$\eta = \frac{\dfrac{E_f}{E_m}-1}{\dfrac{E_f}{E_m}+\dfrac{2l}{d}},$$

where E_c, E_f and E_m are the modulus of composite, fiber (MWNT) and matrix, respectively. v_f is the volume fraction of the fiber. l and d are the length and the diameter of CNT. The Halpin-Tsai equation was originally used for composites with unidirectional reinforcement.

2.2 SHEAR LAG MODEL

This model refines the law to predicting elastic modulus by introducing the effect of the filler aspect ratio. The equation of the elastic modulus of three-dimensional random short fiber composites is as follows [24]:

$$E_c = E_m + v_f\left[\eta_l\eta_T E_f - E_m\right], \tag{2}$$

$$\eta_l = 1/5, \quad \eta_T = 1-\frac{\tanh(\beta r)}{\beta r}, \quad r = 4l/d, \quad \beta^2 = \frac{2\pi E_m}{E_f(1+\nu)\ln(1/v_f)},$$

where ν is the Poisson ratio of matrix, which is equal to 0.35.

2.3 NEW MODEL

This model focuses on a single fiber of length l and diameter d, which is encased in a concentric cylindrical shell of matrix. Length of outer cylinder and CNT are the same. The fiber is aligned parallel to the x-axis. Only the axial load F parallel to fiber is of interest (Fig. 1).

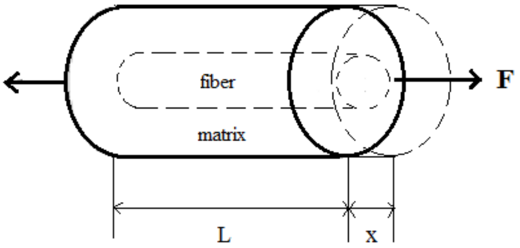

Fig. 1. The force on a cross-section of the nanocomposite element.

We used a linear spring model instead of polymer matrix and CNT, as shown in Fig. 2.

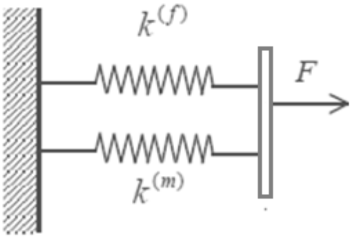

Fig. 2. Arrangement of CNT and matrix.

For this arrangement, loads are not equal

$$F = F_m + F_f = F_m\left[1 + \frac{F_f}{F_m}\right] . \tag{3}$$

Here, F_f and F_m are the corresponding fiber load and matrix load. The equivalent stiffness of CNT and matrix for spring model in Fig. 2 can be obtained from Eq. 4.

$$K_i = \frac{E_i A_i}{L_i} . \tag{4}$$

E_i, A_i and L_i are elastic modulus, cross-section and length, respectively. In this study, the subscripts f and m refer to the fiber and matrix. Because of different properties of component, it can be assumed that the strains on the fibers and matrix in the loading direction are not same

$$\epsilon_f \neq \epsilon_m$$

and

$$\epsilon_m = m\,\epsilon_f , \tag{5}$$

where m is a constant that depends on fiber properties and fiber volume fraction. Using Hooke's law

$$\frac{\sigma_m}{E_m} = m\frac{\sigma_f}{E_f} . \tag{6}$$

Substituting $\sigma = F/A$ in Eq. 6

$$\frac{F_m}{E_m A_m} = m\frac{F_f}{E_f A_f} .$$

Then,

$$\frac{F_f}{F_m} = m\frac{E_mA_m}{E_fA_f}\,. \tag{7}$$

Based on linear spring we have $F = kx$. Substituting in Eq. 3

$$(kx)_c = (kx)_m\left[1 + \frac{F_f}{F_m}\right].$$

We assumed that the displacement of matrix and composite are same,

$$k_c = k_m\left[1 + \frac{F_f}{F_m}\right]. \tag{8}$$

Substituting Eq. 4 in Eq. 8

$$\left(\frac{EA}{L}\right)_c = \left(\frac{EA}{L}\right)_m\left[1 + \frac{F_f}{F_m}\right].$$

Assuming that matrix and composite have equal length, then we obtained the elastic modulus of nanocomposite as follow:

$$E_c = E_m\left(\frac{A_m}{A_c}\right)\left[1 + \frac{F_f}{F_m}\right]. \tag{9}$$

Volume fraction of matrix can be obtained from the following equation:

$$v_{m,f} = \frac{V_{m,f}}{V_c} = \frac{A_{m,f}L}{A_cL} = \frac{A_{m,f}}{A_c}\,, \tag{10}$$

where v_m, v_f and V_c are the volume of matrix, CNTs and composite, respectively. The composite volume fraction is a function of the fiber weight fraction and the densities of the carbon fiber and the matrix [25]

$$v_f = \frac{w_f}{w_f + \left(\frac{\rho_f}{\rho_m}\right)(1 - w_f)}\,, \tag{11}$$

where w_f is the nanotubes weight fraction, ρ_m is the density of the matrix, ρ_f is the density of fibers. Substituting Eq. 7 and Eq. 10 in Eq. 9,

$$E_c = E_m\left(\frac{A_m}{A_c}\right)\left[1 + \left(m\frac{E_mA_m}{E_fA_f}\right)^{-1}\right] = E_mv_m\left[1 + \left(m\frac{E_mA_m}{E_fA_f}\right)^{-1}\right], \tag{12}$$

where m is a constant that depends on fiber properties and fiber volume fraction

$$m = f(L_f, d, v_f).$$

Due to fit the suitable curve to the experimental data, we obtained this equation:

$$m = c\frac{l}{d}v_f^b\ , \tag{13}$$

where l is the length of fiber, d – the average diameter of fiber, b and c are constants of Eq. 13, same for each nanocomposite, which is equal to 1.689. Trough substituting Eq. 13 in Eq. 12, the elastic modulus of composite is

$$E_c = E_m v_m\left[1 + \left(\left(c\frac{l}{d}v_f^b\right)\frac{E_m v_m}{E_f v_f}\right)^{-1}\right]. \tag{14}$$

3 RESULTS AND DISCUSSION

Comparisons are performed between the predictions given this new model, Halpin-Tsai model, and experimental data reported by Montazeri [26], see Fig. 3.

For more comparison, we employed experimental results by Meng et al. [21]. The results are shown in Fig. 4.

Through predicting elastic modulus by using the Halpin-Tsai theory, results shown good agreement with experimental than shear lag theory. The Halpin-Tsai theory has high error in high MWNT weight percent. Through using this new model, results are

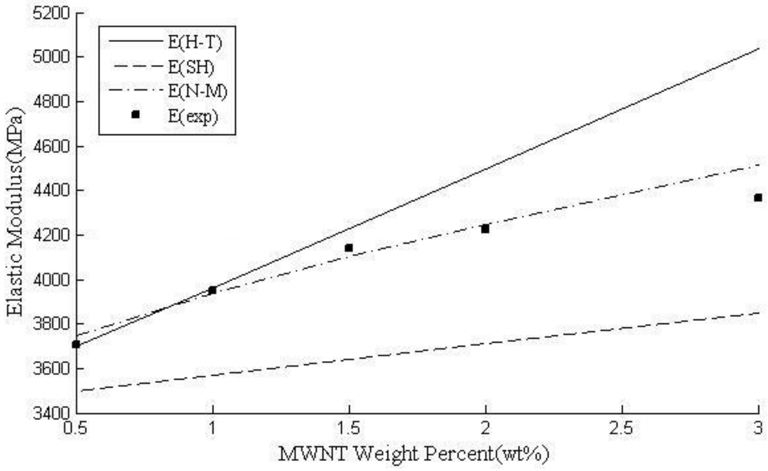

Fig. 3. Relation between elastic modulus of nanocomposite and MWNT weight percent, comparison among experimental data (exp) [26], Halpin-Tsai (H-T), new model (N-M), and shear lag (SH) theory.

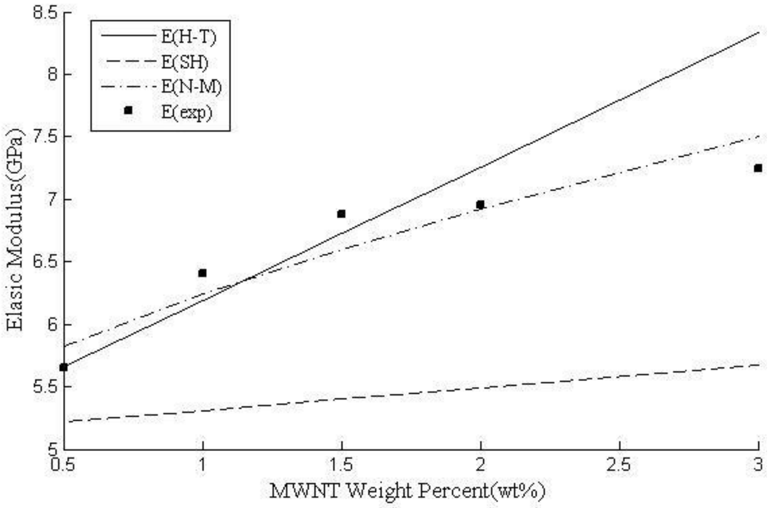

Fig. 4. Relation between elastic modulus of nanocomposite and MWNT weight percent, comparison among experimental data (exp) [26], Halpin-Tsai (H-T), new model (N-M), and shear lag (SH) theory.

improved and error had a decrease than the others in high weight percent. To consider the efficient of length, diameter and weight percent of CNTs on Elastic modulus of nanocomposite, the new model was used. As shown in Fig. 5. Increasing the elastic modulus of nanocomposite is related to increasing on CNTs weight percent and length of CNT and decreasing the diameter of CNT.

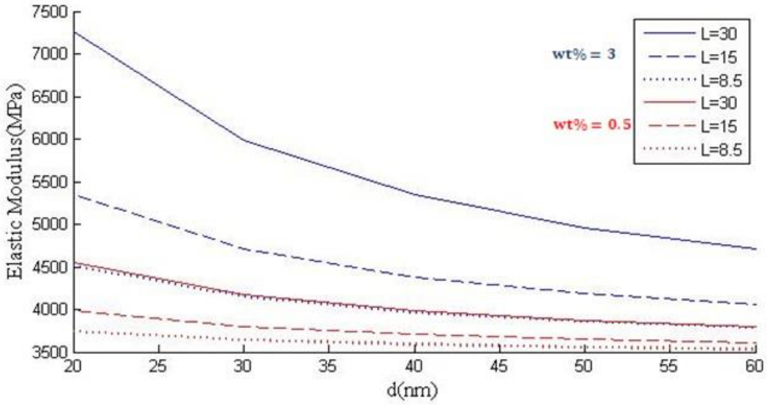

Fig. 5. The efficient of CNTs weight percent, length and diameter of CNT on elastic modulus of nanocomposite.

4 CONCLUSION

To verify the predictions of the new model we used experimental data and some well-known theories. The correlation of the experimentally obtained elastic modulus showed a good agreement with this model. This model is suitable to predict the elastic modulus of nanocomposite with polymer matrix. The effects of length, diameter of CNT and CNT weight percent on the mechanical properties were investigated. Increasing the elastic modulus of nanocomposite is related to increasing on CNTs weight percent and length of CNT and decreasing the diameter of CNT. Through predicting error of elastic modulus by using the other theories, errors at high volume fraction at most of models were more than 10%, while by using this new model we improved the results and error has been decreased.

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