Mechanics of Materials 127 (2018) 48–54

Contents lists available at ScienceDirect

Mechanics of Materials

journal homepage: www.elsevier.com/locate/mechmat

Strength calculation of graphene/polymer nanocomposites using the combined laminate analogy and progressive damage model

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ARTICLE INFO

Keywords:
Nanocomposites
Graphene
Laminate analogy
Progressive damage
Strength

ABSTRACT

In this research, a new model was presented to estimate the strength of graphene/polymer nanocomposites. This model, called “the laminate analogy progressive damage (LA-PD) model”, is a combination of the laminate analogy (LA) approach and a progressive damage model. A nanocomposite was replaced by an equivalent laminated composite (ELC) which contain several isooriented layers. An incremental algorithm was presented to simulate the stress-strain behavior of nanocomposites up to the final failure. First, using the Mori-Tanaka method, the stiffness tensor of the aligned-graphene composite was calculated. Then, using the classical lamination theory (CLT) the elastic modulus of the ELC was obtained. The maximum stress criteria were used to detect the damaged layers. After degrading the stiffness of damaged layers, the elastic modulus of the ELC was updated for the next strain increment. The results show that the tensile modulus and strength increased significantly by increasing the Graphene nanoplatelet (GNP) aspect ratio. However, for aspect ratios higher than about 500, the magnitude of these improvements decreased. A comparison of the results of the present model with the available experimental data in the literature proves the validity of the model.

1. Introduction

GNP due to its extraordinary physical and mechanical properties is known as a potential candidate for the next generation of reinforcing agents of composite materials. Experimental studies have shown that considerable improvements were obtained in the mechanical properties of polymeric resin by adding a very small portion of the GNP (Shokrieh et al., 2014; Song et al., 2011).

In recent years, numerous theoretical studies have been performed to predict the mechanical properties of nanocomposites. The molecular dynamics (MD) (Hu et al., 2005; Gou et al., 2004; Rahimian-Koloor et al., 2018) and molecular structural mechanics (MSM) (Shokrieh and Rafiee, 2010b; Shokrieh and Rafiee, 2010a) methods have been used to model the properties of nanocomposites. As these methods encounter many computational limitations, continuum-based approaches can be used to model such materials. The micromechanical methods are known as continuum-based approaches, which have been mainly used to model the short-fiber and particulate composites. Recently, it has been shown that by some modifications, micromechanical approaches can also be used to study the mechanical properties of nanocomposites (Shi et al., 2004; Seidel and Lagoudas, 2006). Some researchers used the Mori-Tanaka method to investigate the mechanical properties of nanocomposites. In the Mori-Tanaka method, the stiffness tensor of composites is calculated using the Eshelby tensor. This tensor is characterized by the geometry of inclusions (Tsai et al., 2011; Hbaieb et al., 2007). Many other researchers have used the semi-empirical Halpin-Tsai equation to calculate the stiffness of nanocomposites (Cadek et al., 2002; Young et al., 2006; Yeh et al., 2006).

Most of the continuum-based studies have focused on the calculation of the elastic modulus of nanocomposites (Shi et al., 2004; Seidel and Lagoudas, 2006; Tsai et al., 2011; Hbaieb et al., 2007; Cadek et al., 2002; Young et al., 2006; Yeh et al., 2006), whereas there are less continuum-based works in the literature on the strength calculation of nanocomposites (Tserpes et al., 2008; Omidi et al., 2010; Chen et al., 2010; Huang and Rodrigue, 2014; Roy and Srivastav, 2017). Tserpes et al. (2008) used the finite element method to estimate the strength of carbon nanotube-reinforced composites. In their model, a perfect bonding was assumed between the nanotube and the matrix until the interfacial shear stress exceeds the corresponding strength. Then, the nanotube/matrix debonding was simulated by prohibiting the load transfer in the debonded region. Their results revealed that the tensile strength decreased significantly with decreasing the interfacial shear strength, while the stiffness was unaffected. Huang and Rodrigue (2014) used the finite element method to investigate the

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https://doi.org/10.1016/j.mechmat.2018.09.002
Received 19 April 2018; Received in revised form 24 August 2018; Accepted 6 September 2018

effects of particle orientation, strain rate and volume content of carbon nanotube reinforced composites. Their results showed that the strain rate may affect the stresses of the composites, but do not affect substantially the initial elastic modulus whatever the tensile or compressive strain applied. Omidi et al. (2010) proposed a new form of the rule of mixtures which considered the effects of length, orientation, and waviness of the nanotubes in the nanocomposites properties. Chen et al. (2010) carried out the three-level failure analysis of CNT-reinforced composites by combining the shear-lag model and the fracture mechanics. They found that in a strong CNT/matrix interface, the failure mode is converted from the CNT pull-out to the CNT break with an increase in the CNT length, and the fracture toughness drops suddenly during this transition. Roy and Srivastav (2017) proposed a novel technique to model damage and damage evolution in graphene nanocomposites. They assumed that the damage evolution was primarily due to changes in non-bonded interactions at the nanoscale. The unknown coefficients in their model were obtained by a linear regression fit of the nanocomposites stress-strain behavior obtained via molecular dynamics (MD) simulations.

An open-source software has been presented by Talebi et al. (2014) which can simulate the fracture behaviors in solids via semi-concurrent and concurrent multiscale methods. Talebi et al. (2015) also used a concurrent coupling scheme which couple the molecular dynamics to the extended finite element method (XFEM). Using their method, the propagation of the cracks and dislocations were simulated in a three-dimensional space. Hamdia et al. (2017) presented a stochastic method for modeling the fracture of polymeric nanocomposites. In their method, nanoparticles and their surrounding interphase zone and the matrix were modeled using a finite element method. Budarapu et al. (2014) presented a different multiscale method using the coarse-graining technique. The performance of their method was studied through four examples. It was shown that in all examples, the obtained crack patterns are in good agreement with the crack pattern achieved from the fine-scale simulations. Msekh et al. (2018) used a phase field approach to predict the tensile strength and fracture toughness of the exfoliated nano silicate clay epoxy nanocomposites. In their work, the effect of the interphase zones on the tensile strength, and fracture parameters of the nanocomposite were studied and it was shown that the tensile strength was mostly affected by the interphase thickness.

Laminate analogy approach (LA) is another continuum-based method, which was proposed by Halpin and Pagano (1969) and commonly used to obtain the stiffness and strength of random-short fiber composites (Chen, 1971; Shokrieh and Moshrefzadeh-Sani, 2017). In this method, the in-plane random material was treated as a stack of infinitesimally thin unidirectional plies bonded together with different fiber angle orientations. The present authors (Shokrieh and Moshrefzadeh-Sani, 2016) coupled that laminate analogy with the Mori-Tanaka method to estimate the stiffness of the nanocomposites. This model was called MT-LA. The MT-LA method has not been used to calculate the strength of nanocomposites.

In this paper, using the concept of the MT-LA method, a new progressive damage model was developed which could simulate the stress-strain behavior of nanocomposites up to the final failure point. This model is a combination of the laminate analogy (LA) approach and a progressive damage algorithm. The model is called the laminate analogy progressive damage (LA-PD) model. The results obtained by this model were found to be in a good agreement with the experimental results, and thereby the validity of the present model was confirmed.

2. The present model

The present progressive damage model is capable of simulating namely the progressive nature of the failure of GNP/polymer composites. In this model, the randomness of the orientation of GNPs was simulated by equivalent laminated composites (ELC), in which each lamina contains aligned GNPs in different angles. The stress-strain behavior of the ELC from the loading initiation up to the final failure was simulated by the model. In the first step, the stiffness tensor of the aligned-GNP/polymer composite lamina was obtained by the Mori-Tanka method and then using the classical lamination theory the elastic modulus of random-GNP/polymer composites was calculated.

A very small strain ($\Delta\varepsilon$), in each increment number (t), has been applied to the ELC:

$$\Delta\bar{\sigma}^{t} = E_{C}^{t-1}\Delta\varepsilon \tag{1}$$

$$\bar{\sigma}^{t} = \bar{\sigma}^{t-1} + \Delta\bar{\sigma}^{t} \tag{2}$$

$$\varepsilon^{t} = \varepsilon^{t-1} + \Delta\varepsilon \tag{3}$$

where E_{C}^{t-1} and $\bar{\sigma}^{t-1}$ are the stiffness and the average stress of the ELC, at increment number of t-1, respectively. The E_{C}^{t-1} was calculated with the MT-LA method and it will be updated in each increment, proportionate to the damage evolution.

The average stress tensor in the GNPs and matrix were calculated and the damaged layers were detected in each strain increment. Two failure modes were considered, namely matrix failure and GNP deboning. Afterward, the mechanical properties of damaged layers were degraded based on the failure modes.

The stress and strain were calculated in each strain increment (according to Eqs. (2) and (3)) until the matrix was damaged in all layers. The algorithm of the present progressive damage model is shown in Fig. 1. It is noted that $\Delta\varepsilon$ should be chosen small enough until the results converge to a certain value. It was found that for common nanocomposites, the optimum value of $\Delta\varepsilon$ is about 0.001.

It has been shown that the mechanical properties of the nanostructures are affected by the scale effects (Pradhan and Murmu, 2009; Pradhan and Phadikar, 2009; Wang and Wang, 2007). This phenomenon was studied by the molecular dynamic (MD) simulation in some of the previous works of the present authors (Rahimian-Koloor et al., 2018a; Rahimian-Koloor et al., 2018b). The results show that the scale effects are negligible for the graphene larger than 150 nm. In this regards, there are several works in the literature, which tried to model the nanocomposites without considering the nanoscale effects (Tserpes et al., 2008; Liu and Chen, 2003; Shokrieh et al., 2013). By considering these facts, the nanoscale effects have not been considered in the present model.

The assumptions of the present model are:

- Both the GNP and the matrix are linear elastic.
- The macroscopic strain field is identical in all layers.
- The GNPs are randomly distributed and their aspect ratio is identical.
- The effect of waviness of GNPs is neglected.

Different parts of the algorithm, shown in Fig. 1, are explained in detail in the following sections.

2.1. *Stiffness tensor of the aligned-GNP/polymer nanocomposites*

To obtain the elastic modulus of random-GNP/polymer composites via the laminate analogy approach, the first step is to calculate the stiffness tensor of the aligned-GNP/polymer composites. For this purpose, the Mori-Tanaka method as a common way to model nanocomposites (Subramanian et al., 2015; Elmarakbi et al., 2016; Pan et al., 2016) was employed. This method is able to calculate the stiffness tensor of composites with different reinforcement shapes. Furthermore, it considers the effect of the collective interactions of reinforcements.

In the Mori-Tanaka method, a fourth-order strain concentration tensor is defined which relates the reinforcement average strain to the composite average strain as follows:

$$\varepsilon_{r} = \mathbf{A}\colon \varepsilon_{c} \tag{4}$$