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Research paper

Simulation of stiffness of randomly-distributed-graphene/epoxy nanocomposites using a combined finite element-micromechanics method

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ABSTRACT

In this study, a new approach was developed for prediction of the stiffness of polymer nanocomposites with randomly distributed graphene sheets. This approach is a combination of the finite element and micromechanics methods. First, the stiffness of the nanocomposites containing one layer of an aligned nano graphene embedded in a polymer was modeled by using a finite element method. The matrix was considered as a continuum phase and each covalent bond of graphene sheet was simulated by an equivalent structural beam. Nonlinear springs were used as Van der Waals bonds in the interphase region of graphene and polymer. Considering the real size of graphene nano platelets, the numerical simulation of the representative volume element of nanocomposites with a real size aligned graphene sheets embedded in the matrix is not a feasible task. Therefore, in the present research, a new approach was developed to overcome this problem. In this new approach, by using the moduli of different graphene sheets with different sizes embedded in a representative volume element, the moduli of a real size graphene embedded in the matrix were predicted. The results obtained by the finite element method were used by the micromechanics approach in order to consider the effect of the random distribution of graphene sheets in a polymer. By combining these two methods, the stiffness of nanocomposites with randomly distributed graphene sheet was predicted. The result of the model is in an acceptable agreement with the result of conducted experimental program.

1. Introduction

Polymer materials reinforced with nanoparticles have recently received tremendous attention in both scientific and industrial communities due to their extraordinary enhanced properties (Kim et al., 2010; Potts et al., 2011; Geim and Novoselov, 2007; Cho et al., 2006; Tjong, 2006). The structural and mechanical properties of polymers can be improved by reinforcing them with small volume fractions of nanoscale additives such as graphene nano platelets. It has been observed that a single, defect-free graphene platelet could have an intrinsic tensile strength higher than that of any other materials (Zhao et al., 2002). Zeng et al. (2008a) mentioned the limitations of mesoscale or macroscale techniques such as micromechanics and the finite element method (FEM) for modeling of polymer nanocomposites. Therefore, they emphasized the importance of the development of computer modeling and simulation techniques for predicting and designing of material properties of nanocomposites. Various researches (Georgantzinos et al., 2010; Tsai and Tu, 2010; Shokrieh et al., 2012; Shen et al., 2010) have modeled the graphene sheet to characterize its properties. However, modeling of nanocomposites with a random distribution of nanoparticles is much complicated than the modeling of a single nanoparticle. Due to this complexity, most of the studies on nanocomposites presented by different authors (Rahman and Haque, 2013; Awasthi et al., 2009) are devoted to nanocomposites reinforced with few layers of graphene with limited sheet dimensions.

One of the methods used for the prediction of nanocomposites properties is the random multi-scale modeling approach (Zeng et al., 2008b). Using this concept, Shokrieh et al. (2014) have developed a combined molecular dynamics-micromechanics (MD-M) method to predict the stiffness of nanocomposites with randomly distributed graphene in a macro level. Although molecular dynamics simulations yield relatively precise results for the stiffness of nanocomposites, such simulations are very time consuming and only small graphene sheets with limited atom numbers can be modeled. In the present study, by combining the finite element (FE) and micromechanics (M) methods a new approach called FE-M method was developed to estimate the moduli of graphene-based polymer nanocomposites with randomly distributed graphene sheets. To assess the proposed FE-M method,

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experiments were performed and results were compared with those of the present model. The results were found to be in a good agreement; thereby the validity of the proposed method was confirmed. The present model (FE-M) in comparison with the previously developed model (MD-M) is much faster with fairly accurate results.

2. Problem statement

The present model predicts the stiffness of reinforced polymeric nanocomposites by considering the random distribution of graphene nano platelets. The model is a combination of the finite element and micromechanics methods, called as FE-M. The representative volume element (RVE) of nanocomposites with aligned distributed graphene platelets in a polymer is simulated using the FE approach, resulting longitudinal (E_{11}), transverse (E_{22}) and normal (E_{33}) moduli of the RVE in the nano-scale. All these moduli are predicted for a real size graphene platelet in the macro scale by extrapolating the results of the simulation. In the next step, the results obtained by the FEM are used by the micromechanics approach and the randomness of nano platelets is considered. Finally, using the finite element and micromechanics methods the stiffness of nanocomposites with randomly distributed graphene in a polymer in the macro-scale is predicted.

3. Modeling of the RVE

In this section, the detail of the RVE modeling is explained. Fig. 1 shows the RVE of a polymer nanocomposite made of aligned graphene sheets. In the following, the procedure of modeling of the RVE containing a single layered graphene sheet, surrounding polymer, the interphase region between the graphene and polymer and the RVE dimension will be described.

3.1. Single layered graphene sheet (SLGS)

To simulate the behavior of graphene nano platelet within the polymer, an atomistic modeling approach in the nano scale was employed by Tserpes and Papanikos (2005). In their approach, the covalent bonds between the carbon atoms were replaced by equivalent structural beams. Li and Chou (2003) have successfully developed a method that links the interatomic force field constants to sectional stiffness parameters of frame structures. They related the variation of interatomic potential energies to strain energies of equivalent structural beams. The relationships achieved by their method are as follows:

$$\frac{EA}{L} = k_r,\quad \frac{EI}{L} = k_\theta,\quad \frac{GJ}{L} = k_\varphi \tag{1}$$

where k_r, k_θ and k_φ represent the bond stretching force constant, bond bending force constant and bond torsional resistance. Moreover, E, G, A, I, J and L are the Young's modulus, shear modulus, cross section area, second moment of area and polar moment of area of the equivalent beam, respectively. By simplifying above equations, the characteristic of an equivalent beam with a circular cross section was derived in terms of force field constants by Shokrieh and Rafiee (2010):

$$d = 4\sqrt{\frac{k_\theta}{k_r}},\quad E = \frac{{k_r}^2 L}{4\pi k_\theta},\quad G = \frac{{k_r}^2 k_\varphi L}{8\pi {k_\theta}^2} \tag{2}$$

where L is the length (0.142 nm) of the carbon-carbon bond in the graphene lattice. The AMBER force field (Cornell et al., 1995) was used for determining the values of k_r, k_θ and k_φ. These values are listed in Table 1.

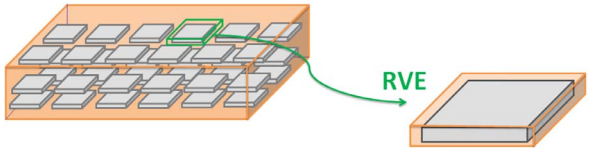

Fig. 1. The RVE of a sample with aligned graphene sheets.

Table 1
The AMBER force field constants.

Parameter	Value
k_r	$6.52 \times 10^{-7}\left[\frac{\mathrm{N}}{\mathrm{nm}}\right]$
k_θ	$8.76 \times 10^{-10}\left[\frac{\mathrm{N\,nm}}{\mathrm{rad}^2}\right]$
k_φ	$2.78 \times 10^{-10}\left[\frac{\mathrm{N\,nm}}{\mathrm{rad}^2}\right]$

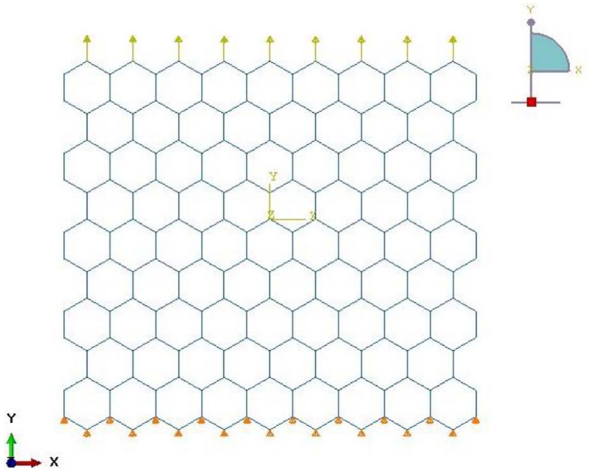

Fig. 2. Graphene sheet under tension.

In the present research, using Abaqus™ software (ABAQUS, 2009), a finite element model of graphene nano platelets was constructed. In order to simulate the graphene sheets, two-node linear beam elements were utilized to replace the covalent bonds with equivalent structural beams. Fig. 2 demonstrates the simulated graphene sheet under tension. By applying the displacement on the top nodes of the graphene sheet, the variation of reaction forces versus displacement was derived.

The results of this simulation are compared with the available results in the literatures in Table 2. The graphene surface Young's modulus (Y) calculated by the present model is in a good agreement with the results presented by other authors. Surface Young's modulus is related to the Young's modulus (E) as follows:

$$Y = E \;.\; t \tag{3}$$

where t is the thickness of the graphene sheet. It should be noticed that changing the direction of loading from the y-axis to the x-axis does not affect the value of the surface Young's modulus of the graphene sheet.

3.2. Surrounding polymer

As mentioned earlier, the polymer in this research is simulated as a continuum phase. Considering the weight fraction of graphene in

Table 2
A comparison of the surface Young's modulus of graphene calculated by the present study and other methods.

Author	Surface Young's modulus (TPa nm)	Graphene thickness (nm)
Sakhaee-Pour (2009)	0.337	0.340
Caillerie et al. (2006)	0.277	N/A
Lee et al. (2008)	0.335	0.335
Reddy et al. (2006)	0.277	0.340
Present study	0.272	0.340