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Finite element modeling of polymer matrix nano-composites reinforced by nano-cylindrical fillers

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ABSTRACT

A new three-dimensional unit cell model has been developed for modeling three constituent phases including inclusion, interphase and matrix. The total elastic modulus of nano-composite is evaluated. Numerical results are in good agreement with the previous proposed theoretical modeling. Higher matrix and inclusion elastic modulus both can dramatically influence the total elastic modulus.

Keywords: *Elastic modulus; Nanocomposites; Polymer; Nano-cylindrical fillers; Modeling.*

INTRODUCTION

The rapidly expanding applications of composite materials in the recent years have provided much optimism for the future of engineering technology. The desire for lightweight and stronger materials encouraged the development of light strength and low ductility materials such as nano-rods reinforced matrix composites. Carbon nano-tubes are of the widely used materials for generating nano-composites [1-4]. The potential mechanical property enhancements have attracted tremendous interest [5-7], since an early research on multi-wall carbon nano-tubes (with a constant interlayer separation of 0.34 A^o) [8] and two years later another study on single-wall carbon nano- tubes [9]. The combination of high elastic modulus, high tensile strength and high aspect ratio (>1000), makes carbon nano-tubes an ideal candidate for reinforcing composite materials [10]. Researchers used the vibration of the nano-tubes as a function of temperature to calculate an elastic modulus of 1 TPa [11]. Common methods to measure the elastic modulus of individual nano-tubes include micro-Raman spectroscopy [12], thermal oscillation [13] and atomic force microscope cantilever [14]. Liu et al. [15] have reported 214% improvement of elastic modulus with incorporating only 2 wt% of multi-wall nano-tubes.

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Considerable efforts have been made in recent years to determine the elastic properties of nano-composites using Finite Element Modeling (FEM) [16-18]. A method for investigating the mechanical response of heterogeneous materials with embedded circular inclusions was demonstrated by Liu & Chiou [19]. The effects of varying the elastic modulus and thickness of the interphase and its effective modulus were analysed by using the commercial software ABAQUS. They found, as might be expected, that the effective elastic modulus depends on the shape and orientation of the inclusions. Moreover, it was found that increasing the interphase thickness would lead to an increase in the effective modulus.

FEM can also be used to evaluate the effect of carbon nano-tubes in composites materials. The Chen & Liu simulation represents the effect of elastic modulus and Poisson's ratios in the transverse plane, using a square matrix with multiple carbon nano-tubes [20]. According to their FEM results, addition of carbon nano-tubes in a matrix at a volume fraction of 3.6%, the stiffness of the composite can increase as much 33%. In addition, Xia et al. [21] have modelled toughening mechanisms in carbon nano-tubes ceramic matrix composites.

In the present study, a three-dimensional unit cell was built in order to investigate the effect of the interphase on nano-composite elastic modulus.

EXPERIMENTAL

Mesh and seed number

A common type of mesh was used in this study; Figure 1 shows an example of a three-phase unit cell sweep meshing technique with hex (inclusion and matrix) and wedge (interphase) element shape. The FEM outcomes should be more accurate as the model is subdivided into smaller elements (the process of dividing a large amount of finite element mesh into sub-regions). The only confident way to know if one has a sufficiently dense mesh is to make several models, changing the seed number and check the discrepancy of one mechanical property such as displacement at the two different seed numbers. From Table 1, it can be concluded that the difference between the results of the last meshes (seed numbers 0.3 and 0.2) are less than 0.4%, thus the further subdivision appears unnecessary. A cylinder was modelled by around 23,000 elements (3267 for inclusion, 1188 for interphase and 18546 for matrix) using a commercial finite element package, ABAQUS 6.4.

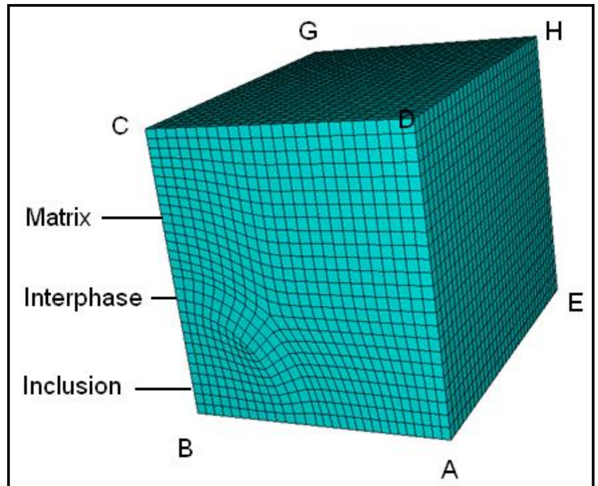

Fig.1. Typical mesh used in the finite element modelling.

Table 1. Minimum displacement with a three-phase cylindrical model

Seed	Inclusion	Interphase	Matrix
2	4.05E-04	1.24E-03	4.55E-03
1	3.87E-04	1.21E-03	4.23E-03
0.9	4.21E-04	1.29E-03	4.29E-03
0.8	4.02E-04	1.24E-03	4.26E-03
0.7	3.91E-04	1.25E-03	4.20E-03
0.6	4.37E-04	1.99E-03	4.25E-03
0.5	4.23E-04	1.17E-03	4.22E-03
0.4	4.18E-04	1.21E-03	4.20E-03
0.3	4.15E-04	1.20E-03	4.21E-03
0.2	4.23E-04	1.20E-03	4.21E-03
0.1	4.24E-04	1.20E-03	4.21E-03

Boundary conditions

The following assumptions were made: nano-rods are uniformly distributed in the matrix, the nano-composite is microscopically homogenous, matrix and nano-rods are isotropic and all three phases are completely tied together. Matrix dimension was taken as 16x16x10 nm^3.

Tensile load is applied via a prescribed displacement onto the face ABCD in the 2-direction; Figure 2, while there are no tractions in other directions thus, the applied shear stresses on all faces of the unit cell is zero. There are six different boundary conditions to calculate by the FEM. Face CDHG and ADHE will remain parallel to the original position after being displaced in the 2-direction, F1=0=F2 and F2=0=F3 for these two faces respectively. Fs represent the normal force acting on faces and are set to zero to simulate a simple unidirectional tension test in the 2-direction. Moreover, all shearing stresses on all boundaries were set to zero. In order to satisfy this requirement, an arbitrary point, which does not belong to any part of the model and is allowed to freely move in any direction was created and related to all nodes on face ADHE. It was found that displacement of all element nodes on this face in 1- direction are the same and equal to that of the arbitrary point [22]. Thus, one can conclude that no external force is applied onto this face. Face EFGH is fixed in 2-direction, U2 = 0 = UR1 = UR2 = UR3 so the displacement on this face is zero. On both the symmetry faces, the symmetry boundary, face BCGF: U1= 0 = F2 = F3 and also face ABFE: U3 = 0 = F1 = F2 were imposed everywhere, since a quarter of cylinder was analysed.

These boundary conditions ensure that the cell, which is a rectangular block of material around the inclusion, remain rectangular and will stack to completely fill the material space. As a result, compatibility requirements between cells are satisfied.

The following analysis was carried out in order to find the elastic modulus "**E**".

$$E = \frac{\sigma_2}{\varepsilon_2} \qquad (1)$$

Where, σ_2 and ε_2 are the stress and the strain in 2-direction. The average value of stress σ_2 is

$$\sigma_2 = \frac{1}{A}\int_A \sigma_y(x,z)d_x d_z \qquad (2)$$

Where, A is the cross section. ε_2 is the strain in 2-direction and can be obtained by:

$$\varepsilon_2 = \frac{\Delta L}{L} \qquad (3)$$

Where, ΔL and L are prescribed displacement and initial length respectively.

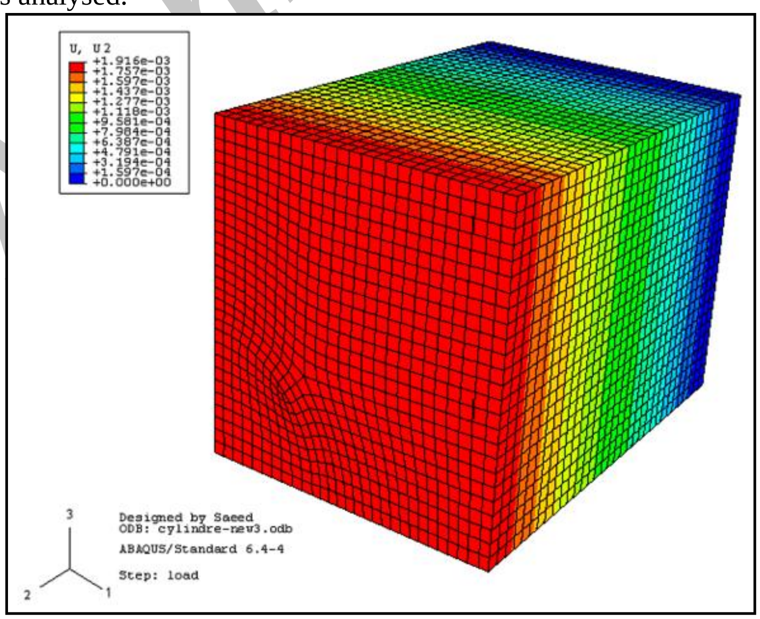

Fig. 2. Simulated displacement distribution in three-phase nano-composite reinforced by cylindrical nano-rods.

RESULTS AND DISCUSSION

Effect of inclusion elastic modulus

From the FEM results in Table 2, the modulus is seen to increase with increasing inclusion elastic modulus as expected from the previously proposed theoretical equation [23]. FEM and theoretical results both reveal that one can increase the elastic modulus of the poor polymer matrix by reinforcing high modulus fillers such as nano-tubes. Interestingly, Li and Chou found that the elastic modulus of the nano-tubes increases as the diameter of the nano-tube is increased [24]. Furthermore, an experimental investigation of the effect of inclusion's length on total elastic modulus was reported by Bai and Allaoui [25]. They evaluated three different lengths of inclusions (1μm, 10 μm and 50 μm). Experimental data shows that the 50 μm length improves dramatically the total elastic modulus compare with others.

Table 2. Effect of inclusion elastic modulus (GPa) on total elastic modulus (GPa)

Inclusion modulus	Nano-composite modulus	
	Theory	FEM
50	5.01	6.32
100	7.73	9.48
150	10.61	12.45
200	13.44	15.43
250	16.29	19.40
300	19.14	22.38
350	21.99	25.35
400	24.85	28.33
450	27.70	32.30
500	30.55	36.28

Note: E_m = 2 (GPa), r_f = 3 (nm), r_i = 3.5 (nm), d_s = 2 (nm), V_f = 0.1 and intragallery enhancement factor = 40

Effect of matrix elastic modulus

In order to study the effect of matrix mechanical properties on total modulus, one must be able to carry out computations with a large range of finite elements. For this purpose, we have chosen the range of 1 to 10 GPa for the polymer matrix. Table 3 shows that finite element results are consistent with the theoretical results and also show good agreement between theoretical and FEM results. It is expected that total elastic modulus increases with increasing matrix modulus.

Table 3. Effect of matrix elastic modulus (GPa) on total elastic modulus (GPa)

Matrix modulus	Nano-composite modulus	
	Theory	FEM
1	2.73	2.80
2	3.74	3.95
3	4.75	5.15
4	5.76	6.30
5	6.77	7.28
6	7.78	8.48
7	8.79	9.67
8	9.81	10.83
9	10.82	11.96
10	11.83	13.21

Note: E_f = 30 (GPa), r_f = 3 (nm), r_i = 3.5 (nm), d_s = 2 (nm), V_f = 0.1 and intragallery enhancement factor = 40

Effect of interphase thickness

In the previous studies, the interphase thickness was considered to be constant at 1 nm. The effect of varying the interphase thickness in determining the total elastic modulus was investigated in this study. A parametric study of the interphase thickness is listed in Table 4.

Table 4. Effect of interphase thickness (nm) on total elastic modulus (GPa)

Interphase thickness	Nano-composite modulus	
	Theory	FEM
5	3.77	4.18
6	3.79	4.36
7	3.81	4.53
8	3.82	4.71
9	3.83	4.87
10	3.84	5.04
11	3.85	5.21
12	3.86	5.38
13	3.87	5.55
14	3.88	5.72

Note: Ef = 30 (GPa), Em = 2 (GPa), rf = 3 (nm), ds = 2 (nm), Vf = 0.1 and intragallery enhancement factor = 40.

As expected from proposed equation [23], total elastic modulus increases with increasing interphase thickness. Interestingly, by adding only 1 nm to the interphase thickness, the total modulus of cylinder model increases 6.5%. Table 4 reveals that total elastic modulus increases sharply to 85 % by adding another 5 nm to the interphase thickness.

Effect of inclusion volume fraction

To investigate the effect of inclusion volume fraction on mechanical properties, cylindrical 3-D three-phase unit cell nano-composites was modelled. Table 5 presents the theoretical and finite element values of elastic modulus from 0% to 14% inclusion volume fraction. Unfortunately, it is well established that adding more than 20% inclusion volume fraction cause reduction in mechanical properties and improvement fails to occur due to chemical interaction between inclusions or low intercalation percentage. Subsequently, neither reduction in mechanical properties was observed from FEM nor from theoretical studies. Thus, analyses were carried out up to only 14% reinforcement volume fraction. Finite element values showed that mechanical properties increase with increase in reinforcement volume fraction as expected from theoretical studies.

Table 5. Effect of inclusion volume fraction on total elastic modulus (GPa)

Inclusion volume fraction	Nano-composite modulus	
	Theory	FEM
0.05	2.82	3.75
0.06	3.00	3.91
0.07	3.18	4.07
0.08	3.36	4.10
0.09	3.55	4.13
0.10	3.74	4.17
0.11	3.93	4.30
0.12	4.13	4.38
0.13	4.33	4.46
0.14	4.54	4.54

Note: Ef = 30 (GPa), Em = 2 (GPa), rf = 3 (nm), ri = 3.5 (nm), ds = 2 (nm) and intragallery enhancement factor = 40

As a result, from the FEM and theoretical results, it can be concluded that mechanical properties in general and elastic modulus in particular increase dramatically below 2-15 wt % inclusion addition.

Note, in this study the finite element modelling has inclusions stacked in neat geometric arrays. This is not so in the real nano-composite and the effect of inclusion randomness is difficult to simulate in FEM models and difficult to include in theoretical models.

CONCLUSIONS

Good agreement has been obtained between theoretical models and the current FEM results of total elastic modulus of nano-composite materials.

Finite element results support the view that the interphase plays a role on the mechanical properties and cannot be neglected.

Theoretical and FEM studies show that total elastic modulus gradually increases with increasing reinforcement volume fraction, contrasting with experimental studies for more than 20 wt% which display decreases.

Analytical magnitudes are quite close to FEM solutions, based on 3-D elasticity, with a difference of about 1.5%. Therefore, the earlier analytical equations may serve as a quick tool to estimate the elastic modulus of nano-composite materials, which are reinforced by nano-rods.

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