MESOMECHANICAL MODEL OF RETICULATE CNT/POLYMER COMPOSITES TO BRIDGE ATOM AND CONTINUUM SCALES

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Summary Mesoscale models for reticulate carbon nanotube (CNT) material as well as the polymer infiltrated reticulated CNT composite are constructed. The reticulate CNT model consists of 9 CNTs, each with length of 100nm, and two gaps are introduced into the CNTs to make the reticulate material a slippage facilitate structure and explore the contribution of the embedded PE chains to the strength of the reticulate CNT composites. The influences of PE adsorption strength are investigated by modifying the Lennard-Jones dispersive parameter as well as the PE chain length. It is shown that stronger reticulate CNT composites can be achieved by inserting shorter PE chains. What's more, the enhancement efficiency is improved when the adsorptions strength of the PE chains are assigned stronger.

INTRODUCTION

Carbon nanotubes (CNTs) possess remarkable mechanical properties for its particular 1D nanoscale structure. However, due to bad desperation of the CNTs and low interaction between the CNTs and the surrounding medium, the enhancement of composites is still far from satisfactory. Consequently, to make the most of the CNT's excellent mechanical and physical properties, considerable attention has been paid to produce novel high-performance macroscale materials by using the CNTs as building blocks, including 1D CNT fibers [1], 2D reticulate CNT films [2].
For 2D reticulate CNT films, it has been theoretically certified that although load can be continuously transferred and the ultimate strengths of the junctions are high, the macroscopic deformation of the reticulate CNT architecture almost comes from the deformation of the CNT mesh in it rather than the effective stretching of the CNTs [3]. Therefore, the failure of the reticulate CNT material is mainly attributed to the slippage between the CNT bundles as well as the deformation of the network rather than axial extension of CNTs. By illustrating epoxy- and poly (vinyl alcohol) in to the reticulate CNTs, reticulate CNT composite with notably higher strength compared to the pure reticulate CNT networks can be fabricated, which implies that the embedded polymer plays an important role of enhancement to the reticulate CNT structures. Therefore, in this paper, mesoscale models of the pure reticulate CNT architecture and the reticulate CNT composites infiltrated with PE chains are built. To make the CNT slippage and PE shearing be the major failure mechanism, gaps are introduced to the CNT bundles. Then the enhancement efficiency of the PE chains with different length and adsorption strength are studied.

METHODOLOGY

For the CNTs, by reproducing the full atomistic results of single CNT tensile load cases, a mesoscopic model with specific parameters was developed, in which the time and length scales are not accessible to the full atomistic model but still includes information about the mechanics of individual CNTs [4].
The reticulate CNT model consists of 9 CNTs, each 100 nm in length with two gaps introduced into every CNT, as illustrated in Fig.1. Among the free space short PE chains with length of 2nm are infiltrated. After the optimized model obtained, the end beads of each nanotube are constrained, as shown in Fig.2.

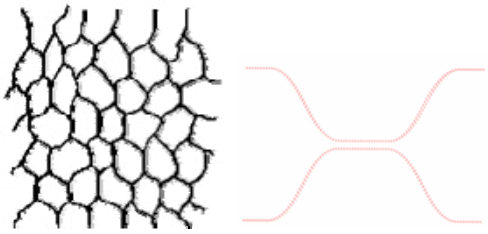

Fig.1 Mesoscopic model of reticulate CNT

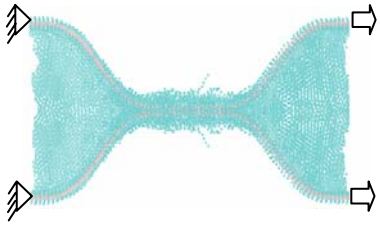

Fig.2 Reticulate CNT /polymer composites

The method in deriving parameters for a mesoscale bead-type model of CNTs from the full atomistic calculation is based on a principle of energy conservation between full atomistic and coarse–grain potentials. The mesoscale model is represented by a function of the total energy of the system expressed as

$$E_{\text{system}} = E_{\text{T}} + E_{\text{B}} + E_{\text{pairs}} \tag{1}$$

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where E_T is the energy stored in the bonds due to axial stretching, E_B is the energy stored in the bonds due to bending, and E_{pairs} is the energy due to weak pair interaction between unbounded beads. For the present model, the functional forms of bonded energy is given as

$$E_T = \frac{1}{2}k_t(r-r_0)^2, \quad E_B = \frac{1}{2}k_\theta(\theta-\theta_0)^2 \tag{2}$$

where k_t and k_θ are the stiffness constants for the bond length and bond angle potentials, respectively, and r_0 and θ_0 are the equilibrium bond length and bond angle, respectively. The non-bonded or Van der Waals interactions are given by a Lennard-Jones potential as

$$E_{pair} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \qquad r \le r_c \tag{3}$$

where r is the distance between two atoms, σ is the distance at zero energy, and ε is the energy well depth. The cutoff distance r_c is taken as 30 Å. Table 1 gives the values for all of the constants used in the interatomic potential.

Table 1 material constants used in mesoscale model

Parameter	Units	CNT-CNT	PSE-CNT	PE-PE
r_0	Å	5.00	--	5.00
k_t	kcal mol $^{-1}$ Å^{-2}	2000	--	2.1
θ_0	Degrees	180	--	180
k_θ	kcal mol $^{-1}$ rad^{-2}	14300	--	4.2
ε	kcal mol $^{-1}$	15.1	10.5	0.8365
σ	Å	10.35	5.8	4.7

RESULTS AND ANALYSIS

The influences of PE chain length are investigated as well as adsorption strength modifying the Lennard-Jones dispersive parameter ε. The tensile test is then repeated using these modified parameters.

The maximum stress σ^* of the PE infiltrated reticulate CNT is normalized by the σ^*_{pure} in a pure reticulate CNT and plotted in Fig.3. The normalized virial stress indicates that stronger reticulate CNT composites are achieved by filling short 1.5 nm PE chains. What's more, the difference becomes greater when the adsorptions between the PE are assigned stronger by multiplying the L-J dispersive parameter ε.

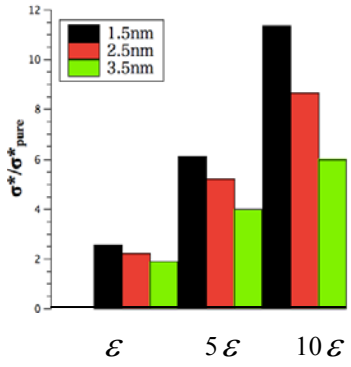

Fig.3 The stress improvement σ^*/σ^*_{pure} under different PE chains length and absorption strength

CONLUSIONS

This paper proposed a mesomechanical model to investigate the enhancement of properties for reticulate CNT/polymer composites. The present model bridges the atom and continuum scales. It is found that the reticulate CNT slippage and PE shearing are the major failure mechanism of the composites. The enhancement efficiency depends on the length and adsorption strength of the PE chains in the composites.

References

[1] Liu K., Sun Y.H. and et al.: Carbon nanotube yarns with high tensile strength made by a twisting and shrinking method. *Nanotech* **21:** 045708, 2010

[2] Ma W.J., Liu L.Q., and et al.: High-strength composite fibers: realizing true potential of carbon nanotubes in polymer matrix through continuous reticulate architecture and molecular level coupling. *Nano Lett* **9:** 2855-61, 2009.

[3] Liu X., Yang Q.S. and et al.: Molecular mechanics modelling of deformation and failure of super carbon nanotube networks. *Nanotech* **22:** 475701, 2011

[4] Buehler M. J.: Mesoscale modeling of mechanics of carbon nanotubes: Self-assembly, self-folding, and fracture. *J Mater Res* **21:** 2855-69, 2006.