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Evaluation of elastic properties of multi walled carbon nanotube reinforced composite

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ABSTRACT

Exceptional mechanical properties like high strength, stiffness and aspect ratio exhibited by carbon nanotubes, make them ideal reinforcements for nanocomposites. In this paper load transfer in multi-walled carbon nanotube (MWCNT) composites is studied under tension and compression loading conditions. Continuum mechanics model is used to evaluate the effective material properties using a representative volume element (RVE) approach. Numerical results are obtained using Finite Element Modeling (FEM) and these results have been validated with rule of mixture results. FEM results are found to be quite closer to the results obtained from rule of mixture. In the present work we have considered a range of matrix material, the range covers the matrix material from metal to polymer, i.e. taken in a form of the ratio of effective modulus of elasticity of CNT to that of matrix material E^t/E^m from 5 to 200. With the addition of the multi-walled CNT in a matrix at the volume fractions of 5.1%, the stiffness of the composite is increased by 46% for compressive loading and 14.9% for tensile loading, as compared with that of the matrix in the case of long CNT at $E^t/E^m = 10$. Multi-walled carbon nanocomposite are found to provide better value of young's modulus in compression as compared in tension, this is due to the higher inter-tube load transfer in compression.

Comparative evaluation of material properties with single walled carbon nanocomposite is also done. It is established that multi-walled carbon nanotube composite provide a better resistance against compression as compared to single walled carbon nanotube composite. Effect of change in diameter and length of multi-walled carbon nanotube on stiffness of nanocomposite have also been investigated. Longer multi-walled carbon nanotubes are found to be more effective in reinforcing the composite as compared to shorter ones. FEM results are also found to be in close approximation with the experimental results, which validates the current model.

1. Introduction

Since the discovery of carbon nanotubes in 1991 [1], they have attracted the attention of scientists and stimulated their imagination in various technological fields. Carbon nanotubes possess novel and unique properties such as low density, extremely high stiffness, resilience, and strength [2–5]. These properties of Carbon nanotubes (CNTs) makes it an excellent reinforcement material for nanocomposites. It has been demonstrated that with just 1% (by weight) of CNTs added in a matrix, the stiffness of the resulting composite can increase between 36% and 42% and the tensile strength by 25% [6]. Experiments and atomistic simulations have been carried out and it is established that CNTs really have an extremely high modulus e.g., [7–9], and a strength around 100 GPa that is significantly higher than the few GPa of the carbon fibers. Apart from these properties, they have high geometric ratio, stiffness-to-weight, and strength-to-weight ratios. These properties can be best exploited by incorporating the nanotubes into some form of matrix, to create nano-composites [10,11]. Polymer matrix has been mostly used, but interest in other matrix materials, such as ceramics and metals is also found. TEM image of MWCNT–Polystyrene composite in which the nanotubes are homogeneously distributed in the polystyrene matrix is shown in Fig. 1 [12].

Carbon nanotubes can be effectively used in preparing nano composites because of their ability to homogeneously disperse throughout the matrix. The improvement in mechanical properties of a composite relies mainly on an effective load transfer mechanism between the composite matrix and the nanotubes. If the adhesion between the matrix and the CNTs is not strong enough to sustain high loads, the benefits of the high tensile strength of CNTs are lost. Sufficiently strong interfacial bonding has been reported for some polymers [13,14]. Andrews et al. [15] produced PS/MWCNT composites by shear mixing, found that the tensile

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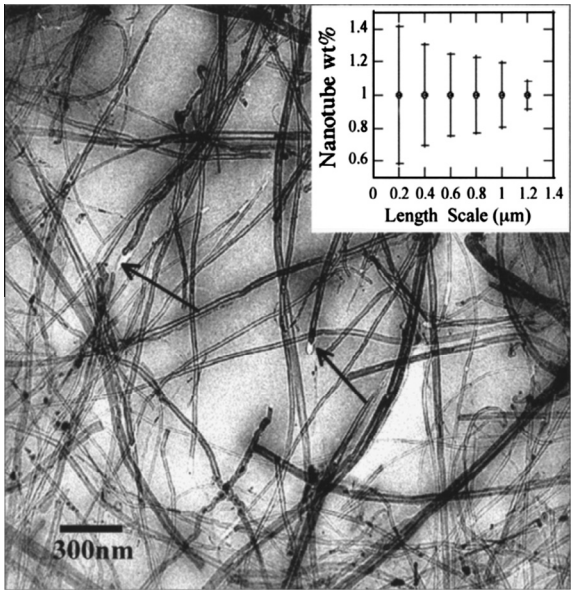

Fig. 1. TEM image of MWCNT–Polystyrene film in which the nanotubes are homogeneously distributed in the polystyrene matrix [12].

modulus increases by only 15% for 5% volume fraction of MWCNTs in matrix. Xia et al. [16] prepared some propylene/CNTs composites where a good dispersion was obtained using a new process to reach the nano-mechanic pulverization.

Computation of the material properties including mechanical, thermal, and electrical properties is a challenging task for producing and designing a novel nanocomposite. The computational approach can be divided into two methods, i.e. molecular dynamics (MD) and continuum mechanics based methods. The MD has yielded many simulation results to understand the behavior of individual and bundled CNTs. Either computational power or numerical algorithm for the MD has been improved rapidly. However, the MD is still limited to simulation of a system containing 106–108 atoms for the period of a few nanoseconds, that is very small length and time scales. The MD simulation has difficulties in handling nanocomposites with large length and time scales. Therefore, the simulation for larger systems or longer time is currently left to continuum mechanics method. The continuum mechanics approach has been applied successfully for simulating the mechanical responses of individual carbon nanotubes, which are treated as beams, thin shells, or solids in cylindrical shapes [17–22]. A 3D solid model for CNTs reinforced composites has been characterized by Liu and Chen [22,23], which ensures the accuracy and compatibility between CNTs and matrix in the composite. The current results using the continuum approaches have indicated that continuum mechanics can be applied to models with dimensions of a few hundred nanometers and larger where averaging of material properties can be done properly for CNTs.

In this paper mechanical properties of multi-walled carbon nanocomposites are investigated using a 3D representative volume element (RVE).The continuum model is composed of MWCNT in form of cylindrical tubes surrounded by matrix material. A range of matrix material is considered varying from polymer to metal matrix. Equations based on the elasticity theory for extracting the effective material properties from solutions of the cylindrical RVEs are derived and numerical studies using the FEM are conducted. Validation of FEM results is done with the analytical results obtained from rule of mixture. Also, the FEM results are compared with experimental results.

2. Modeling and simulation

A homogeneous and elastic model of cylindrical RVE filled with a transversely isotropic material is considered as shown in Fig. 2. CNT and matrix are considered to be perfectly bonded at the interface. Axial stretch and axial compression loading conditions are considered using cylindrical RVE to evaluate the material constants in axial direction. The general 3-D strain–stress relation relating the normal stresses ($\sigma_x,\ \sigma_y,\ \sigma_z$) and strains ($\varepsilon_x,\ \varepsilon_y,\ \varepsilon_z$) for a transversely isotropic material can be written as:

$$\begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \end{Bmatrix} = \begin{bmatrix} \frac{1}{E_x} & -\frac{\upsilon_{xy}}{E_x} & -\frac{\upsilon_{zx}}{E_z} \\ -\frac{\upsilon_{xy}}{E_x} & \frac{1}{E_x} & -\frac{\upsilon_{zx}}{E_z} \\ -\frac{\upsilon_{zx}}{E_z} & -\frac{\upsilon_{zx}}{E_z} & \frac{1}{E_z} \end{bmatrix} \begin{Bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{Bmatrix} \tag{1}$$

In this uniaxial load case, shown in Fig. 3, the stress component on the plane $Z = L/2$, E_z is obtained as $\sigma_x = \sigma_y = 0, \varepsilon_z = \frac{\Delta L}{L}, \varepsilon_x = \varepsilon_y = \frac{\Delta R}{R}$.

$$E_z = \sigma_z/\varepsilon_z = L/\Delta L\sigma_{ave} \tag{2}$$

where, the averaged value of stress is given by

$$\sigma_{ave} = \frac{1}{A}\int_A \sigma_z(x, y, L/2)dxdy$$

with 'A' being the area of the end surface. σ_{ave} can be evaluated for the RVE using the FEM. From Eqs. (2) and (3) we get

$$\varepsilon_x = -\frac{\upsilon_{zx}}{E_z}\sigma_z = -\upsilon_{zx}\frac{\Delta L}{L} = \frac{\Delta R}{R} \tag{3}$$

Thus, obtains an expression for the Poisson's ratio:

$$\upsilon_{zx} = -(\Delta R/R)/(\Delta L/L)$$

Eqs. (2) and (3) can be applied to estimate the effective Young's modulus E_z and Poison's ratio ($\upsilon_{zy} = \upsilon_{zx}$), once ΔR and the stress σ_{ave} in load case is obtained.

The FEM results obtained from Eq. (2) are compared with the results obtained from simple analytical expressions, or rules of mixtures (Section 3), based on the strength of materials theory.

2.1. Simulation of Van der waal forces

In case of a MWCNT, there exists non covalent interaction between the individual shells of MWCNT. That can be adequately described by a weak van der Waals force using the Lennard–Jones potential [24]

$$V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{4}$$

In Eq. (4), the terms σ and ϵ are defined as the Lennard–Jones parameters, r is the distance between interacting atoms. For a Carbon–Carbon non-covalent interaction, the values of the

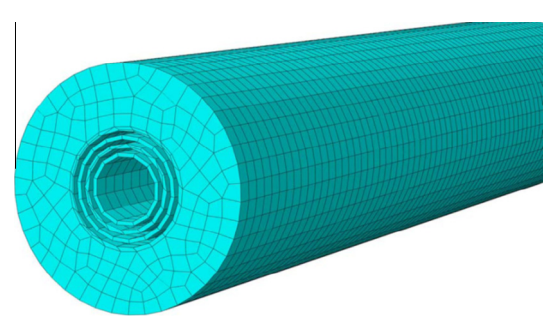

Fig. 2. Long multiwalled carbon nanotube through the length of cylindrical RVE.