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Analysis of alignment effect on carbon nanotube layer in nanocomposites

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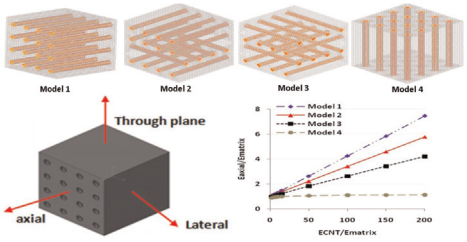
HIGHLIGHTS

- Different layer formations are analysed for double walled carbon nanotube (DWCNT) composites.
- Parallel, perpendicular and vertical alignments of DWCNT layers are considered in the matrix material.
- Four composite models with different combinations of DWCNT layers are constructed.
- Variation in axial, lateral and through plane properties of composites is observed for different alignments.
- Higher value of axial stiffness of composite is observed, when the fibers are aligned in direction of loading.

GRAPHICAL ABSTRACT

Effect of various alignments of double walled carbon nanotubes (DWCNT) in composite is evaluated for axial, lateral and through plane properties.



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ABSTRACT

In this work, effect of various alignments of double walled carbon nanotubes (DWCNTs) in composite is evaluated for axial, lateral and through plane properties. Layers of DWCNTs are incorporated in the matrix. Four models with different layer combinations are analysed using 3D representative volume element. The highest value of axial modulus is observed for composite in which DWCNTs are aligned in direction of loading. Enhancement in lateral stiffness is observed for the models in which layers are aligned in plane perpendicular direction. Through plane stiffness is improved in vertically aligned DWCNT composite. It is observed that both axial and lateral moduli of composite behave non-linearly with respect to DWCNT volume fraction. This is because of the effect of agglomeration, due to the higher content of DWCNT in the composite. The proposed simulation is based on the experimentally adopted alignment of carbon nanotubes. DWCNT based composites with specific properties along various directions can be designed by controlling the volume fractions and alignment of the DWCNT sheets.

1. Introduction

Carbon nanotubes (CNTs) exhibit unique atomic structure with interesting properties such as high strength, high modulus, high aspect ratio and low density [1–4]. Due to this unique combination of properties, they have emerged as an excellent tailoring agent in the preparation of multifunctional composites. A lot of researches

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have been done on polymer, metal, ceramic matrix based nanocomposites [5–10]. It has been revealed that the reinforcement effect of carbon nanotube on matrix depends not only by their content within the hosting system but also by the level of dispersion, alignment of fibres and load transfer between fibre and matrix. Cha et al. worked in CNT/metal composite and obtained homogeneous distribution of CNTs using the molecular level mixing method. As a result they observed more than 200% increase in yield strength [11]. It is found that, significant enhancements in both the modulus and strength of nanocomposites can be achieved with the alignment of nanotubes due to the improvement in load transfer between the polymer matrix and the CNT reinforcement [12]. The main advantage for fibrous composite materials in structural applications is that the material can be "tailored" by proper alignment of the fibers in the various layers so as to optimize the desired structural behavior. Usually the fibres are strong in longitudinal direction but weak in the lateral direction. Therefore, when they are used to make structural composites, the final product will have weak through-the-thickness mechanical properties. Zhao et al. found that the dispersion of CNTs increases young's modulus, ultimate tensile strength, and storage modulus of composites loaded by 30%, 25%, and 10%, respectively, compared with the neat epoxy [13]. Deterioration in modulus is observed with the increase in filler loading, if agglomeration of CNTs occurs [14].

Experimental techniques are very informative but costly at the nano-scale. Whereas computational approaches being cost effective are also used for modeling nanostructures. The computational methods used are molecular dynamics, continuum mechanics and combination of both the techniques [15,16]. Liu et al. simulated the process of pulling out carbon nanotube from polyethylene by inlaying the carbon nanotube into polyethylene using molecular dynamics [17]. Panchal et al. reported dynamic responses of single walled boron nitride nanotube by constructing an atomistic model based on finite element method [18,19]. In continuum approach, macroscopic behavior is studied assuming that the material is continuously distributed throughout its volume. Based on continuum mechanics, using the representative volume element (RVE), Liu et al. evaluated the effective mechanical properties of CNT-based composites [20,21]. The boundary element method, based on boundary integral equation (BIE) formulation, was also used to solve the boundary integral equations governing the rigid-inclusion problem [22]. The MD simulation has difficulties in handling nanocomposites with large length and time scales. Therefore, the simulation of larger systems is currently left to the continuum mechanics method.

In this work, axial, lateral and through plane properties of double-walled carbon nanotube (DWCNT) based composites are evaluated. Four different models are constructed using 3 dimensional RVE. Parallel, perpendicular and vertical alignments of DWCNTs are considered in the models.

2. Modeling

2.1. Simulation of models

Four different models are constructed based on 3 dimensional RVE. Each model consists of different combination of DWCNT layers in the composite. Solid elements (8 noded), shell elements (4 noded) and spring elements are used in the modeling of composite. Spring elements are used to simulate the van der waal forces between adjacent walls of DWCNT. The material of DWCNT and matrix is considered as homogeneous and transversely isotropic.

According to elasticity theory, uniaxial stress and strain are given by

$$\sigma = \frac{F}{A}, \qquad F = \sum_{i}^{n} F_i$$

$$\epsilon = \frac{\Delta L}{L}$$

Elastic modulus obtained using the stress and strain values

$$E = \sigma/\epsilon = \sigma L/\Delta L \tag{1}$$

where σ is the compressive stress of RVE in the loading direction, and ϵ is the strain of RVE in loading direction. F and ΔL are the load and displacement in loading direction. F_i is the reaction force of the ith node, i is the node number, A is the section area, and L is the length of the numerical specimen.

2.2. Simulation of van der Waal forces

The interaction between the walls of DWCNT is described by weak van der Waal forces using the Lennard–Jones potential. Linear spring elements whose stiffness is determined by equivalent force concept are used to simulate the interlayer van der Waals force as reported in [23].

According to the Lennard–Jones potential [24], the inter-wall pressure dependent on inter-wall separation distance, as determined by Zhao and Spain [25] is given as

$$p(d) = \frac{\Psi}{6}\left[\left(\frac{d_0}{d}\right)^{10} - \left(\frac{d_0}{d}\right)^{4}\right] \tag{2}$$

Here $p(d)$ is the interlayer pressure, d the inter-layer distance, $\Psi = 36.5$ GPa, $d_0 = 0.34$ nm the Lennard–Jones constant which is the distance between walls in equilibrium. The pressure inter-wall separation relation is shown in Fig. 1. Linearizing Eq. (2), taking variation of the increment of distance $d - d_o$ near the equilibrium position almost linear, as shown in Fig. 1. Let $\varphi = d/d_0$, (2) can be rewritten as

$$p(\varphi) = \frac{\Psi}{6}\left[(\varphi)^{-10} - (\varphi)^{-4}\right] \tag{3}$$

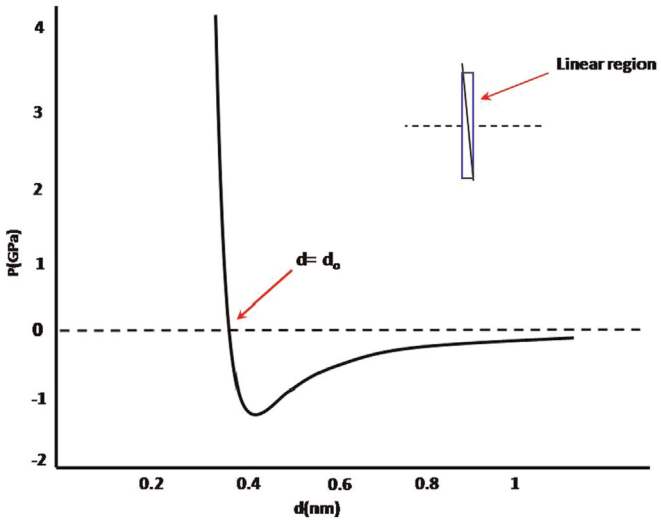

Fig. 1. The relation between interlayer pressure and layer distance.