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Multiscale modeling for mechanical properties of carbon nanotube reinforced nanocomposites subjected to different types of loading

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ABSTRACT

Multiscale modeling was presented for the nonlinear properties of polymer/single wall carbon nanotube (SWNT) nanocomposite under tensile, bending and torsional loading conditions. To predict the mechanical properties of both armchair and zigzag SWNTs, a finite element (FE) model based on the theory of molecular mechanics was used. For reducing the computational efforts, an equivalent cylindrical beam element was proposed, which has the unique advantage of describing the mechanical properties of SWNTs considering the nonlinearity of SWNT behavior. For a direct evaluation of the rigidities of the proposed equivalent beam, the data obtained through atomistic FE analyses of SWNT were fitted to six different equations, covering the three types of loading for both armchair and zigzag configurations. The proposed equivalent beam element was then used to build a cylindrical representative volume element (RVE) using which the effects of the interphase between SWNT and the polymer on the mechanical properties of RVE could be studied. It was found that while the interphase has a small effect on the nanocomposite stiffness, the ratio of (SWNT length)/(RVE length) dramatically affects the nanocomposite stiffness.

1. Introduction

Carbon nanotubes (CNTs) [1] have attracted substantial attention in the scientific community [2–4] in the recent decades, owing to their remarkable mechanical, electrical and thermal properties [5]. The CNT reinforced nanocomposites have also been the subject of extensive research studies [6,7]. For example, Qian et al. [8] showed that the addition of 1 wt.% (i.e. 1% by weight) multiwall carbon nanotube to polystyrene resulted in 36–42% and ~25% increases in the elastic modulus and the break stress of the nanocomposite properties, respectively. In addition, Yokozeki et al. [9] reported the retardation of the onset of matrix cracking in the composite laminates containing the cup-stacked CNTs compared to those without the cup-stacked CNTs.

The properties of the CNT reinforced nanocomposites depend on a variety of parameters including CNT geometry and the interphase between the matrix and CNT. While the experimental studies in nanoscale are often expensive and difficult, the theoretical methods are still employed extensively. For example, the mechanical and fracture behavior of CNTs have been investigated using the method of molecular mechanic in different studies [10–16]. Li and Chou [17] used beam-type members to model the C–C bonds and determined the modulus of elasticity and shear modulus of SWNT. The sectional property parameters of these beam members were obtained by establishing a linkage between the structural mechanics and the molecular mechanics. Li and Chou [17] verified their model by simulating the modulus of a sheet of graphite (around 0.995–1.033 TPa) successfully. Tserpes et al. [18] proposed an atomistic-based progressive fracture model for simulating the mechanical properties of CNTs by considering the initial topological and vacancy defects under axial loading. They made use of the FE method to analyze the nanotube structure and the modified Morse interatomic potential to simulate the non-linear force field of the C–C bonds. The effect of one-vacancy defect was also studied by Meo and Rossi [19]. In another study, Rossi and Meo [20] proposed a FE model of SWNTs based on the molecular mechanics theories. They examined SWNT under axial loading to evaluate mechanical properties such as the Young's modulus and the ultimate strength. However, the load–displacement curve of C–C bonds is often considered linear. For instance, Papanikos et al. [21] combined an atomistic-based FE analysis with the fundamental concepts of mechanics of materials in order to evaluate the geometrical characteristics and elastic properties of the beams that possess the same tensile, bending and torsional behavior as CNTs. They assumed a linear behavior for the load–displacement relation of the C–C bonds, which makes the presented results acceptable just for small strains in SWNT.

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Nomenclature

a, b	constant coefficients
A_{eq}	cross sectional area of equivalent beam element
A_{RVE}	cross sectional area of RVE
d_n	SWNT diameter
D_e	dissociation energy
D_{eq}	average diameter of equivalent beam element
D_{ij}^e	the energy required to stretch the bond from its equilibrium distance to infinity
$E_{eq,ax}$	axial modulus of equivalent beam element
$E_{eq,be}$	bending modulus of equivalent beam element
E_m	matrix modulus
E_n	SWNT modulus
EA	tensile rigidity of SWNT
EI	bending rigidity of SWNT
F	force of atomic bonds
F_a	axial reaction force of SWNT
$F_{RVE,ax}$	axial reaction force of RVE
$F_{RVE,be}$	transverse reaction force of RVE
$F_{RVE,tor}$	tangential reaction force of RVE
F_{tr}	transverse reaction force of SWNT
F_φ	tangential reaction force of SWNT
G_{eq}	shear modulus of equivalent beam element
GJ	torsional rigidity of SWNT
I_{eq}	second moment of inertia of equivalent beam element
I_{RVE}	second moment of inertia of RVE
J_{eq}	polar moment of inertia of equivalent beam element
J_{RVE}	polar moment of inertia of RVE
k_e	force constant at the minimum of the well
L_e	distance between the end of RVE and end of SWNT
L_n	SWNT length
L_{RVE}	RVE length
M	momentum of atomic bond
n	SWNT chirality
r	the distance between carbon atoms
r_0	the bond equilibrium length
R_n	SWNT radius
R_{RVE}	the outer radius of RVE
t_{eq}	thickness of equivalent beam element
t_n	thickness of SWNT
u_a	axial displacement of SWNT
$u_{RVE,ax}$	axial displacement of RVE
$u_{RVE,be}$	transverse displacement of RVE
u_{ta}	tangential displacement of SWNT
u_{tr}	transverse displacement of SWNT
V_{el}	electrostatic interaction component of potential energy
V_r	the C–C bond stretching component of potential energy
V_{vdw}	the van der Waals interaction component of potential energy
V_θ	the C–C–C bond angle bending component of potential energy
$V\varphi$	the C–C–C bond dihedral angle torsion component of potential energy
V_ω	the inversion terms of component of potential energy
β	a fitting parameter
γ	shear strain of SWNT
ε	SWNT tensile strain
ε_b	C–C bond strain
θ	bending angular deformation
θ_c	C–C bond angular deformation
υ_m	matrix Poisson's ratio
υ_n	SWNT Poisson's ratio
φ_n	the angle of twist of SWNT
$\varphi_{RVE,tor}$	the angle of twist of RVE
Δr_{ij}	C–C bond length variation

The continuum approaches have recently received more attention because of their reduced computational expenditure. While, continuum approaches have been used in some studies to model the sole CNT [22], this method has also been found very helpful in modeling the nanocomposites. For example, Pantano and Cappello [23] investigated the effects of CNT curvature and its interface interaction with the matrix on the nanocomposite stiffness using a nano-mechanical analysis. Shokrieh and Rafiee [24] replaced an embedded carbon nanotube in a polymer matrix with an equivalent long fiber for predicting the mechanical properties of the carbon nanotube/polymer composite in order to predict the mechanical behavior of the CNT/polymer composites. Hu et al. [25] analyzed the elastic deformation of a representative volume element (RVE) under various loading conditions and evaluated the macroscopic elastic properties of the CNT reinforced nanocomposites. Tserpes et al. [26] proposed a multiscale RVE for modeling the tensile behavior of SWNT reinforced nanocomposites in which a perfect bonding was assumed between the nanotube and the matrix until the interfacial shear stress exceeded the corresponding strength. In [26], a beam element represented SWNT in RVE but it was applicable only for tensile loading condition. In addition, some researchers used numerical methods to verify the micromechanical models [27,28].

Almost all of the equivalent structural models proposed in the past for SWNTs have been based on a linear relationship for the interatomic potential of the carbon-atoms, which makes them inappropriate for modeling either large strains or the breakage of SWNTs. In this paper, a FE model of SWNTs based on a molecular mechanics theory, which accounts for nonlinear relationship for the interatomic potential, is proposed. Using the proposed model, the rigidities of both armchair and zigzag SWNTs under axial, bending and torsional loading are determined. The effects of length and diameter of SWNT on its rigidities are also studied. The data obtained from FE analyses are then fitted to six equations in order to provide direct estimates for the rigidities of both armchair and zigzag SWNTs. Using these equations, an equivalent cylindrical beam is introduced. Afterwards, the FE method is used for modeling the matrix and building a RVE that contains the proposed equivalent beam element. The effects of interphase between SWNT and the matrix configuration of RVE on the modulus of the resulted nanocomposite are also studied.

2. Finite element modeling

2.1. Molecular mechanics theory

To model SWNT, it was assumed that SWNT acts like a 3-D frame, in which the C–C bonds are the load bearing elements and the atoms are the joints. The FE method was used to analyze the SWNT structure and the modified Morse interatomic potential was used to describe the nonlinear behavior of C–C bonds. In its general formula, the potential energy (Fig. 1) is described as

$$V = \sum V_r + \sum V_\theta + \sum V_\varphi + \sum V_\omega + \sum V_{vdw} + \sum V_{el} \qquad (1)$$

where V_r, V_θ and V_φ are the potential energies related to the bond stretching, the bond angle bending and the dihedral angle torsion. Similarly, V_ω is associated with the inversion terms, V_{vdw} the van der Waals interaction and V_{el} the electrostatic interaction. Depending on the materials and loading conditions, different functions can