Composites Communications 2 (2016) 9–14

Contents lists available at ScienceDirect

Composites Communications

journal homepage: www.elsevier.com/locate/coco

Characterizing the strength and elasticity deviation in defective CNT reinforced composites

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ARTICLE INFO

Keywords:
Carbon nanotube reinforced composites
Atomic vacancy defects
Multiscale modeling
Effective elastic properties
Representative volume element

ABSTRACT

In this paper, the Multiscale 3D Representative Volume Element approach is proposed for modeling the elastic behavior of carbon nanotubes reinforced composites with vacancy defects. The Carbon Nanotube has been modeled using atomistic scale by Molecular Structural Mechanics. Space frame structure similar to 3D beams and point masses are employed to simulate the discrete geometrical constitution of the single walled carbon nanotube. The covalent bonds between carbon atoms found in the hexagonal lattices are assigned elastic properties using beam elements. The nodes are treated as Carbon atoms on which the point masses are applied. The vacancy defect is considered in the single wall carbon nanotubes. The matrix phase has been investigated using continuum mechanics approach at macro scale level. The carbon nanotube and matrix regions are connected by interfacial zone using beam elements. Using the proposed multi scale model, the deformations obtained from the simulations are used to predict the elastic modulus of the nanocomposite. The mechanical properties are evaluated for various Vacancy defect locations and number of defects. The influence of the vacancy defects on the chiral CNT reinforced composite is studied under an axial load condition. Numerical equations are used to extract the effective material properties for the cylindrical RVE with non-defective CNTs. The FEM results obtained for non-defective Carbon Nanotubes are consistent with analytical results for cylindrical Representative Volume Element, which validate the proposed model.

1. Introduction

Due to the extraordinary properties, carbon nanotubes have been used in many diverse areas of applications. Exceptionally high stiffness, strength, resilience and superior electrical as well as thermal properties make Carbon nanotubes, the ultimate reinforcing materials for an entirely new class of Nanocomposites. Carbon nanotubes are discovered first by [7]. The specific tensile strength of a single layer of a multiwalled carbon nanotube can be as high as 100 times that of the steel, and the graphene sheet is as stiff as diamond at low strain. With such special properties, carbon nanotubes have a vast amount of applications in the fields of materials, electronics, field emission, biology, medicine and electrochemistry. Using fracture mechanisms of Nanocomposites, (Ayatollahi et. al. [19]) experimentally proved that even by adding 1 wt% of nanoparticles like CNT and CNF, the impact strength of nanocomposite increases by 19% and 13% respectively.

This paper focuses on carbon nanotube reinforced composite materials. Similar to any of the man-made materials, carbon nanotubes are also susceptible to various kinds of defects. It has been revealed that defects in nanotubes including vacancy defects, metastable atoms, pentagons, heptagons, heterogeneous atoms, discontinuities of walls, distortion are commonly present in CNTs, [1,8]. The molecular dynamics simulations is developed and compared with micromechanics model to investigate the effective interface concept, as a characteristic phase, which describes the particle size effects thermoset epoxy-based nanocomposites, [14].

A method has been proposed to characterize the internal mechanical behavior of the intermediate media in terms of the nanoparticle size, and the nanophysics of the intermediate media by [3]. A continuum model through the matching of homogenization and deformation energy to a full atomic molecular model is used to numerically obtain the mechanical response. The effect of nanosilica contents on mechanical properties of the epoxy matrix was studied by [13], using macroscopic experiments and nanoscale simulation. Also the weak interface toughening and strengthening mechanism of nanocomposites was presented using simulation.

A discrete nonlinear finite-element approach has been reported [15] to determine the mechanical properties of individual carbon–carbon (C–C) bonds. They have shown that the homogeneous elastic properties of the defective nanotubes can be qualitatively and quanti-

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http://dx.doi.org/10.1016/j.coco.2016.09.006
Received 30 June 2016; Received in revised form 7 September 2016; Accepted 10 September 2016
Available online 24 October 2016

tatively different from the pristine configurations. It is also reported that, defective nanotubes show a slight reduction in axial stiffness, but large variations of Poisson's ratio depending upon locations of vacancies for isotropic material.

Extensive Monte Carlo based numerical simulation has been used to simulate the individual C–C bonds. The bonds are simulated as Beam elements. Also the MM based fracture analysis [16] has been done for SWCNT, where beam elements are used to represent the covalent bonds and nonlinear characteristics of the beam elements are obtained using the modified Morse potential. They have predicted that, failure stress and strain values of vacancy defected SWCNTs are respectively 27% and 52% smaller than those of pristine ones.

For nanoscale systems, the volume fraction of defects becomes significantly high because the overall size of the system is in nanometers. Defects degrade the mechanical performance of Carbon Nanotubes, since they alter not only their inelastic properties but also the elastic properties, such as the Young's modulus and Poisson's ratio. The longitudinal and transverse stiffness as well as the flexural rigidity in tension, torsion and bending are, consequently, being altered. Therefore, it is necessary to investigate the effects of such defects on the properties of nanocomposites.

2. Simulation model

A vacancy defect is one which leads to the removal of one atom and the three bonds related to it, located at the center and at different positions along the length of the carbon nanotube. The modeling of the defect is performed during the creation of the FE mesh where the necessary modifications in the nanotube lattice are made. The demonstrated space frame model utilizing the Molecular Structural Mechanics approach has the ability to consider vacancy defects at multiple positions. To model the defects, necessary modifications in the nanotube lattice are made. After constructing the space frame structure, to model the non-reconstructed one vacancy and two vacancy defects, carbon atoms and related bonds are removed from the nanotube structure. Every carbon atom neighboring a vacancy has one dangling bond and is coordinated by two other atoms apart from the vacancy. The C–C bond lengths in the two-hold coordinated carbon atoms are shorter than the regular C–C bond length by 0.03–0.04 Å.

As used by other researchers [17,18] Von-Mises criterion has been used for strength evaluation for nanocomposites. This suggest that the current simulations completely support the strength evaluation criterion and hence can be considered for evaluating feasibility in terms of strength considerations.

2.1. Atomic structure of carbon nanotubes

An atomistic finite element model, [9], consisting of beam elements and concentrated masses is used to study the Single walled Carbon Nanotube reinforced composites. Fig. 1 represents the finite element mesh of cylindrical RVE based nanocomposite.

The interatomic covalent forces between carbon atoms are used to evaluate the elastic properties of the beam elements. The atomistic finite element model is presented, using total strain energy of the system. The system assumes small deformations and electrostatic interactions are neglected, [5].

$$\zeta_{total} = \sum \zeta_s + \sum \zeta_B + \sum \zeta_T \tag{1}$$

ζ_s is the bond stretching energy, ζ_B is the bond angle bending energy, and ζ_T is the bond torsional energy which can be expressed as:

As the potential energy in the approaches of molecular mechanics and structural mechanics are independent, energy equivalence of the stored energy is given as, [12].

$$\frac{EA}{L} = k_R,\ \frac{EI}{L} = k_\theta,\ \frac{GJ}{L} = k_\phi \tag{2}$$

The elastic properties of the beam elements are given as:

$$d = 4\sqrt{\frac{k_\theta}{k_R}}, E = \frac{k_R^2 L}{4\pi k_\theta}, G = \frac{k_R^2 k_\phi L}{8\pi k_\theta^2} \tag{3}$$

where d, L, E and G represent the diameter, length, Young's Modulus and Shear Modulus of the beam element. As CNT is considered as a space frame structure in this analysis, the beam element length is taken equal to the distance of the covalent bond between two carbon atoms in the graphene sheet. The radius of the carbon atoms, neglecting the radii of the carbon nuclei, is taken as 2.7×10^{-5} A. Mass of the carbon nuclei, which is positioned at the end of each beam element, is considered as 1.99×10^{-26} kg. In this analysis, it is assumed that the masses of the electrons are not significant in comparison with the nuclei.

2.2. Modeling of matrix phase

The matrix phase is modeled using Continuum mechanics approach based on the concept of a representative volume element. The matrix phase is assumed as linearly elastic, isotropic and homogenous materials, with given Young's modulus and Poisson's ratio. The inner radius of matrix is kept equal to the nanotube radius plus half of the wall thickness of the tube. The solution of a continuum problem by the Finite Element Method (FEM) involves the field variable, which possesses infinitely many values, as it is a function of each generic point in the body or solution region. The quadratic solid (brick) elements are employed in the 3-D models, which offer higher accuracy in FEM stress analysis.

For uni-axial load case, as shown in Fig. 2 the stress component on the plane Z=L/2: Ez is obtained by:

$$\sigma_x = \sigma_y = 0, \epsilon_z = \frac{\Delta L}{L} \text{ and } E_z = \frac{\sigma_z}{\epsilon_z} = \frac{L}{\Delta L}\sigma_{ave} \tag{4}$$

where, the averaged value of stress is given by:

$$\sigma_{ave} = \frac{1}{A}\int_A^a \sigma_z(x, y, L/2)\,dxdy \tag{5}$$

2.3. Modeling of interface

Interface behavior in nanocomposites greatly affects the elastic properties. Interfaces can either be modeled as a continuum or as a discrete structure. In the case of interfaces between two phases of composite material, the primary interest is to study the load transfer between the phases across the interface. The load transfer phenomenon depends on the strength of the interface of composites. The effects of interfacial strength on the stiffness and load transfer of composites have been studied by using various design parameters. To characterize the discrete interfacial elements at the nanoscale dimensions, the nodes are generated on RVE. The beam elements are employed as the interfacial connecting elements with defined stiffness.

These beam elements connect the atoms of the nanotube radially with corresponding nodes which correspond to the inner cylindrical surface of the matrix, which is meshed using finite elements. The length of the beam element is taken as $t_n/2$, [6]. Thus, the proposed model simulates the interfacial region using discrete beam elements.

2.4. Rule of mixtures (ROM) for nanocomposites

To evaluate the effective material properties for composites, a simple analytical expression, named Rule of Mixtures is used. It is based on strength of materials theory. This concept along with some extended results in the case of fiber reinforced composites has been successfully applied in the past for carbon nanotube based nanocomposites using different Representative Volume Elements [11,2]. All the