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Analysis of elastic properties of carbon nanotube reinforced nanocomposites with pinhole defects

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ABSTRACT

Due to their unique molecular structure, carbon nanotubes exhibit outstanding properties. They are regarded as ideal reinforcements of composites. In this paper, the effects of pinhole defects on mechanical properties are investigated for wavy carbon nanotubes based nanocomposites using 3-D Representative Volume Element with long carbon nanotubes. The carbon nanotubes are modeled as continuum hollow cylindrical shape elastic material with pinholes, having some curvature in its shape. These defects are considered on the single walled carbon nanotubes. The mechanical properties like Young's modulus of elasticity are evaluated for various values of waviness index, as well as type and number of pinhole defects. The effects of interactions between both defects as well as their influence on the nanocomposites are studied under an axial loading condition. Numerical equations are used to extract the effective material properties for the different geometries of Representative Volume Elements with non-defective carbon nanotubes. The finite element method results obtained for non-defective carbon nanotubes are consistent with analytical results for cylindrical Representative Volume Elements, which validate the proposed model. It is observed that the presence of pinhole defects as well as waviness, can significantly reduces the effective reinforcement, when compared with nanotubes without pinhole defects and this reinforcement decreases with the increase of the number of pinhole defects.

1. Introduction

Carbon nanotube (CNT) is an ultimate example of small-size, ultra strength material. Due to their remarkable properties, carbon nanotubes have been employed in many diverse areas of applications. Iijima discovered the carbon nanotubes in 1991 [1]. CNTs possess exceptionally high stiffness, strength and resilience, as well as superior electrical and thermal properties, which makes it the ultimate reinforcing material for the nanocomposites. Especially, it has been addressed that the carbon nanotube has outstanding Young's modulus and tensile strength and is one of the most promising materials with potential as an ultimate reinforcing material in the nanocomposites [2–4]. The various mechanical properties of nanotubes [5–9] have been extensively studied.

Very small diameter, large aspect ratio, extremely high strength and stiffness naturally make the CNT to become a kind of most attractive 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% [10]. The mechanical-load carrying capacities of CNTs in nanocomposites have also been demonstrated in experiments [10,11] and preliminary simulations [12,13]. The measured specific tensile strength of a single layer multi-walled carbon nanotube can be as high as 100 times that of steel and the graphene sheet (in-plane) is as stiff as diamond at low strain. These mechanical properties motivate further study of possible applications for lightweight and high strength materials [14]. Very interesting and unexpected change of Poisson's ratio from positive to negative is observed in the design of sheet-derived composites. *Usually when materials are pulled in one direction, they get thinner in the other direction. But the specially designed carbon nanotube sheets can increase in width when stretched. They can also increase in both length and width when uniformly compressed. The composites made from such sheet are called 'sheet derived composites'. The negative in-plane Poisson's ratio is associated with such composites and explains the phenomena of biaxial sheet expansion.* The mechanical property optimization using mixtures of nanotubes has been presented [15] for continuous tunability of Poisson's ratio, modulus, strength, toughness, density, and electrical conductivity of nanotube sheets.

However, there are many parameters, which may influence the mechanical properties of nanocomposites, such as the dispersion, alignment, waviness and defects of CNTs. Similar to any of the many man-made materials used today; CNTs are also susceptible to various kinds of defects. The nonlinear behavior is fully described [16] for the entangled carbon nanotubes model. This

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entanglement is due to the bending of the coil tips produced by the ball impact. Experimental observations have revealed that, topological defects are commonly present in CNTs [17]. *The defect in continuum media is defined as a space region containing the discontinuity of the order parameter like line defect in 3D and point defect in 2D. The topological defect is the singularity in the continuum that cannot be removed by continuous deformation of the local region in the vicinity of the singularity. If the topological defect is encircled by the closed continuous loop, the value of the order parameter changes by an integer value, called the winding number.*

Defects degrade the mechanical performance of CNTs, 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 these factors on the macroscopic properties of composites. Hirai et al. [18] have shown that in the case of the defective single walled carbon nanotubes (SWCNT), the yield tensile strength decreases to about 80% that of the non-defective SWCNT by a single type 1 pinhole defect. The Halpin–Tsai concept has been applied for simulating the mechanical responses of various composites under different boundary as well as loading conditions [19]. This concept can also be applied successfully for carbon nanotubes based nanocomposites. CNTs are treated as solids in cylindrical shapes with Representative Volume Element (RVE), which is employed to study the interactions of the nanotube with the matrix, to investigate the effective material properties of the nanocomposites [20] and validated by Halpin–Tsai equations. However, work has been found on the effect of defects on buckling of CNTs [21], where the influence of two types of pinhole defects was studied on the buckling strength of SWCNTs and significant reduction in buckling properties was observed due to the presence of large pinhole defects. Effect of single atomic vacancy defects on the buckling of SWCNTs has been studied using Molecular Dynamics (MD) and continuum beam models [22]. Here the effect of carbon nanotubes curvature on the nanocomposite stiffness is also investigated using nanomechanical analysis. Brinson et al. proposed that using finite element analysis and micro-mechanical methods, it was proposed that observed curvature of embedded CNTs or waviness significantly reduced their reinforcement capabilities compared to straight CNTs [23,24]. Often Halpin–Tsai model [25] is used for aligned, discontinuous fiber reinforcement, which approaches the rule of mixtures for large values of E_t/E_m and l/d like 100 and 500 respectively. An effective l/d of the CNT deduced from such analysis, can explain the stress transfer phenomena in CNTs [26]. The concept of unit cells or Representative Volume Elements has been applied in this paper to study the CNT based composites at the nanoscale.

In this unit cell or RVE approach, a single nanotube with surrounding matrix material can be modeled, with properly applied boundary and interface conditions to account for the effects of the surrounding materials. Evaluation of effective elasticity property has been done for non-defective long as well as short CNTs with hexagonal RVE under an axial stretch [27]. It is found that both the waviness and debonding can significantly reduce the stiffening effect of the CNTs. The effective moduli are very sensitive to the waviness and this sensitivity decreases with the increase of the waviness [28]. Shady and Gowayed have discussed the impact of the nanotube curvature on the elastic properties of nanocomposites using the modified fiber model and the Mori–Tanaka approach [29]. Lin et al. have worked on thin Ni films with various thicknesses on polished MgO (1 0 0) single crystal substrates [30]. The structure formation with pinholes array in the film was discussed in terms of the elastic strain energy. In the current work, the coupled effects of multiple defects such as pinhole and waviness in CNTs are investigated for the nanocomposites stiffness. Analytical equations given by Halpin–Tsai are used to extract the effective material properties for the cylindrical and hexagonal RVEs with CNTs under axial loading condition.

2. Simulation model

Simulation model based on Halpin–Tsai model [19] is used to evaluate the mechanical properties of CNT based nanocomposites. These equations are very user friendly forms of self consistent model of composite materials as shown in Eq. (1). Basically Halpin–Tsai equations are the set of empirical relationships, which enable the properties of composite materials to be expressed in terms of the properties of the matrix and reinforcing phases together with their proportions and geometry. Such a generalized self-consistent model of a composite is assumed with a composite cylinder model in which the embedded phase consisted of continuous and perfectly aligned cylindrical fibers and each fiber to behave as though it is surrounded by a cylinder of pure matrix; outside this cylinder lays a body with the properties of the composite. Both materials are assumed to be homogeneous and elastically transversely isotropic about the fiber direction. Halpin–Tsai equations were curve fitted to exact elasticity solutions using the parameter ζ. The factor ζ is used to describe the effect of geometry of the reinforcing phase on a particular property, which may differ for different properties in the same composite. The properties of a composite can be determined by the Halpin–Tsai equation as given below. Eq. (1) will be used to verify the FEM results of the effective longitudinal modulus.

$$\frac{E_z}{E_m} = \frac{1 + \varepsilon\alpha\phi}{1 - \alpha\phi} \tag{1}$$

$$\alpha = \frac{E_t/E_m - 1}{E_t/E_m + \varepsilon} \tag{2}$$

E_t and E_m represent the elasticity moduli of the CNT as well as matrix phase respectively, along the longitudinal direction. Under the uniaxial load case, the elasticity modulus component over the plane $Z = L/2$ is obtained as:

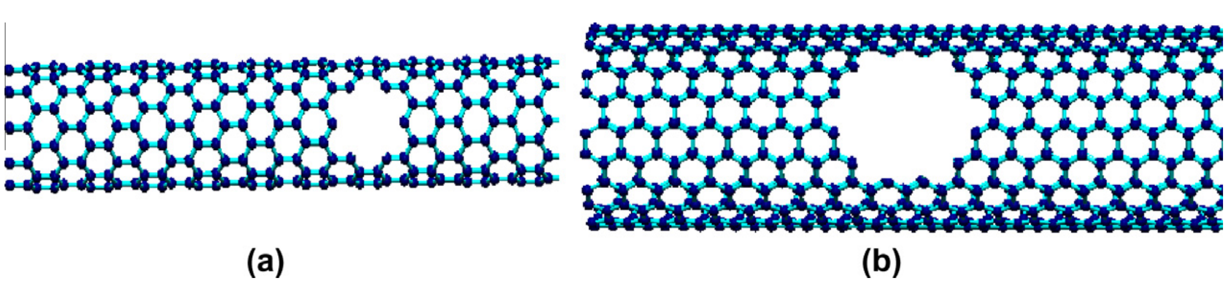

Fig. 1. (a) Schematic view of a single pinhole defect model. Type 1: defect of six atoms. (b) Schematic view of a single pinhole defect model. Type 2: defect of 24 atoms.