

Stress mapping around SWNT and MWNT in polymer-matrix nano-composites

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Objectives:

The objective of this research is to evaluate the stress distribution in nano-composite materials manufactured from single and multi-wall nano-tubes (SWNT and MWNT). We plan to utilize and modify some of the models available in archived literature to cross the scale-gap between the atomic scale presented by the nano-tubes, and the continuum scale presented by the matrix material. We will also attempt to introduce a new approach to map the stresses distribution around nano-tubes and link it to failure mechanisms encountered in various loading regimes.

Relevance to Center Mission:

The proposed research work expands on the basic knowledge needed to enhance our understanding of the behavior of nano-composite materials manufactured by adding nano-tubes to polymer materials. Such addition can introduce substantial improvement to the physical properties of the polymer such as higher strength and modulus, better dimensional stability, higher thermal stability and heat distortion temperature, better flame retardancy and reduced smoke emissions, better electrical conductivity, etc. In order to fully utilize the potential of such unique materials a comprehensive understanding of their response is necessary which can help expand the application of nano-composites in various fields such as biomaterials for tissue repair, thin film capacitors, automotive parts, blades and food packaging.

State of the Art:

Carbon nano-tubes (CNTs) are graphitic sheets rolled into seamless tubes in which carbon atoms are in a periodic hexagonal arrangement. They can have single or multiple layers of carbon atoms in the thickness direction in the form of concentric cylinders with closed caps at both ends. CNTs received much attention since their discovery [1-3] due to their superior mechanical properties. Studies showed that the deformation of a SWNT is completely reversible within 4% strain [4-7] and can sustain a 5% compressive strain prior to buckling and even larger strain under torsion [8].

Many studies have addressed the mechanical properties of carbon nano-tubes, either experimentally [9-11] or numerically [12-14]. Pan reported the average Young's modulus and tensile strength of MWCNTs with 12 nm inner diameter, 30 nm outer diameter and length of about 2 mm as 0.45 ± 0.23 TPa and 1.72 ± 0.64 GPa, respectively [10]. Nakajima et al. used a hybrid nanorohotic manipulation system inside a scanning electron microscope (SEM) and a transmission electron microscope (TEM) to measure Young's modulus of a carbon nano-tube and reported it as 1.23 TPa [11]. Analytically, Kalamkarov et al. modeled the behavior of carbon nano-tubes using two different approaches, namely analytical-asymptotic homogenization and a numerical-structural mechanics based FEA approach [12]. The Young's modulus and shear modulus for SWNT predicted using the first approach are 1.71 TPa and 0.32 TPa, while the second approach predicted them as 0.9–1.05 TPa and 0.14–0.47 TPa, respectively [12]. Meo and Rossi [13] developed a FEA model using nonlinear and torsional spring elements to evaluate the mechanical properties of single-walled nano-tubes using different nano-tubes chirality. The average Young's modulus was reported as 0.92 TPa.

Researchers have also analyzed carbon nano-tubes using theoretical modeling [15, 16] following one of two approaches: i) an atomistic approach which uses classical molecular dynamics [4, 17], tight bending molecular dynamics [18] and density functional theory [19]. This approach requires huge computational undertaking and limits the practical application of this approach to systems that contain a small number of atoms, and ii) a continuum mechanics approach with a focus on energy balance such as the work done by Tersoff [20] and Ru [21, 22].

Due to their outstanding mechanical properties, CNTs can be used effectively as reinforcements in nano-composite materials [23, 24]. Compared to graphite fibers with 300-800 GPa Young's modulus and about 5 GPa tensile strength, nano-tubes have better properties as well as surface area per unit volume leading to a much larger nano-tube/matrix interfacial area which affects the modulus and fracture behavior of their composites [25-27]. Using 0.5 wt% of CNTs increased the Young's modulus of epoxies up to 200% and the tensile strength up to 140% [28, 29]. Therefore it is necessary to understand the effective elastic properties of CNTs to explore the potential application of using them as structural reinforcement in nano-composite materials.

The most significant parameters that affect the properties of nano-composites are the uniform dispersion of the nano-tubes and their alignment in the matrix. The strong attractive interaction between nano-tubes causes them to aggregate. Additionally, the high surface area of nano-tubes, especially in cases of high loading levels, increases the viscosity of the mixture and causes their dispersion to be extremely difficult. Recent research works have shown the possibility of obtaining well-dispersed and well-aligned nano-tubes in nano-composites by functionalizing their surfaces to enhance their compatibility with the matrix [30-32]. Jia et al. used a radical initiator to open the π -bonds and create C-C bonds between the CNTs and the polymer to improve their dispersion efficiency [30]. Park et al. used sonication during in-situ polymerization of the monomers to enhance the dispersion efficiency of nano-tubes [31]. Walters et al. suspended SWNT segments in a strong magnetic field and then filtered them out of suspension while they remain aligned to enhance their alignment in nano-composites [32].

Numerous micromechanical models have been developed to evaluate the macroscopic mechanical properties of composites reinforced with carbon fibers, however, it is not easy to implement the same methodologies for nano-composites due to the significant scale difference between nano-tubes and carbon fibers. As a result, new modeling strategies have been proposed to calculate the overall mechanical properties of nano-composites. Two approaches are typically followed: i) utilize molecular mechanics to model the interaction between the matrix and nano-tube and construct a homogeneous equivalent continuum model for the nano-tube surrounded by a cylindrical volume of a polymer matrix [33]. Classical micromechanics analysis is then implemented to calculate the effective bulk properties of the equivalent continuum model, and ii) an array of nano-tubes embedded into a polymer matrix is modeled using lattice dynamics [34]. A series of self-similar concentric cylinders are used to construct the overall model of a micro-fiber having a specific orientation. These two approaches were compared in terms of assumptions and validity of ranges and both had consistent results in calculating the elastic properties of the nano-composites [35].

A number of studies based on continuum modeling were conducted to evaluate the interfacial shear strength of SWNTs nano-composites. Wagner modified Kelly-Tyson approach assuming uniform interfacial shear and axial stresses to evaluate the interfacial shear behavior [36]. Li and Chou developed a model to characterize the interfacial shear stress transfer from the polymer to the nano-tubes utilizing a molecular structural mechanics approach [37, 38]. For both models [36, 38], the nano-tubes were considered as cylinders (i.e. free of caps). Gao and Li developed a shear lag model using two concentric cylinders to represent a nano-tube surrounded by a matrix [39] ignoring the effect of surrounding nano-tubes. Jiang et al. modified Cauchy-Born rule to establish a constitutive model to study the effect of CNT radius on the mechanical behavior. They integrated the standard cylindrical equilibrium equation over the CNT thickness to obtain the equilibrium equation for a SWCNT and study the effect of the radius of the nano-tubes on tension and pure torsion. Results showed that the change in radius has a minor effect on the mechanical behavior [40].

Based on the understanding presented in the few paragraphs above, many critical questions remain unanswered. What is the stress distribution in the matrix around the nano-tube and how is it affected by neighboring nano-tubes? How does the stress distribution change from the body to the cap regions? What is the role of such stress distribution on the failure mechanisms of nano-composites and how is it manifested?

Approach:

We propose to construct a robust and easy-to-implement approach to model the stress distribution around nano-tubes in nano-composite materials and their mechanical response. Since micromechanical approaches cannot be directly applied at the nano-level, atomistic simulation will be used to model the materials' behavior. Connecting the atomistic model to continuum models gives the ability to describe the mechanical behavior of the nano-composites and map the stresses and strains in their vicinity.

At the atomic level, a portion of the nano-tube will be represented by a truss structure, in which every pin-joint represents an atom and every truss-member represents a bonded or a non-bonded interaction between the atoms. A virtual strain is applied at the pin-joints and used along with the elastic properties of the truss elements and its dimensions to calculate the strain energy of the truss as a whole. A similar volume of graphite with isotropic properties will be considered to have equivalent strain energy under the same displacement, as shown in Figure 1, which allows the calculation of its elastic properties (Young's modulus, and Poisson's ratio) similar to the work done in [45]. The level of accuracy of this approach was confirmed by Wu et al. [46] for nano-tubes with diameters more than 1.6 nm. Such equivalence of strain energy, under similar displacements, allows the connection between atomistic and continuum models.

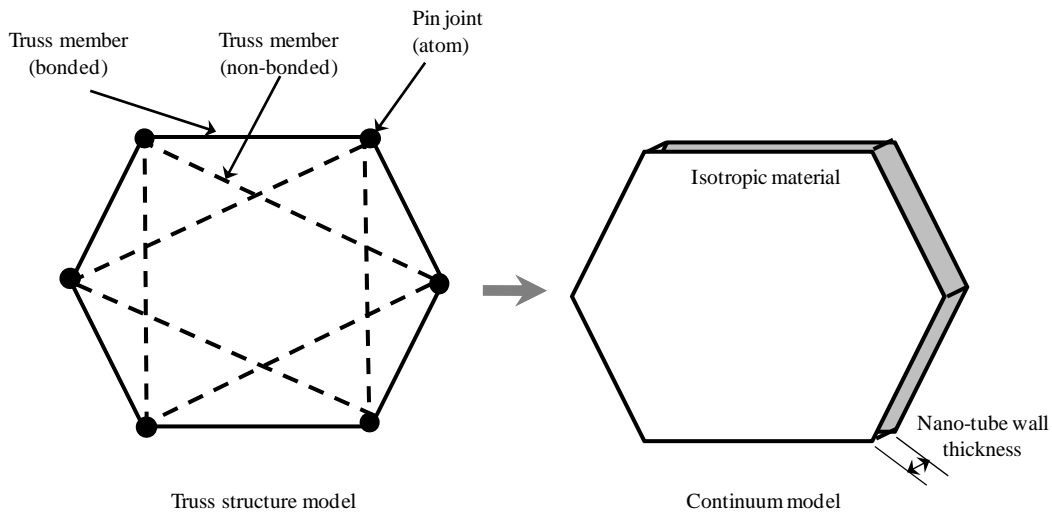


Figure 1: A schematic representation of mapping of atomistic scale response to continuum modeling.

The stress distribution under tensile and shear forces will be mapped around the nano-tube in both longitudinal and transverse directions of the nano-tube. The shear-lag theory will be used to model the nano-tube in the longitudinal direction while the modified Mukhelishvili complex potential will be used for the transverse direction including the effect of neighboring nano-tubes [47]. The interfacial shear stress on the nano-tube/polymer matrix interface will be investigated utilizing the stress mapping approaches.

Nano-composite material will be manufactured utilizing functionalized carbon nano-tubes (SWCNT and MWCNT) to improve bonding with common structural resins, such as epoxies, and enable stiffer and tougher composites. Mechanical tests of the nano-composites, including tensile, short beam shear and 4-point bending, will be conducted. The spatial distribution of nano-tubes within the matrix will be determined using an Atomic Force Microscope (AFM). The model will calculate the stress-strain response for different tests, utilizing the spatial distribution of nano-tubes reported by the AFM observation, and compare it to experimental data.

One question, at least, clearly remain unanswered: how can the stress distribution around the nano-tubes calculated by the proposed model be experimentally verified? Can data acquired from pure flexure conditions, in 4-point bending, or shear, from short beam shear, be adequate for such purpose? We hope that an answer to this question and others be possible as the research progresses.

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