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Nanocomposite material properties estimation and fracture analysis via peridynamics and Monte Carlo simulation

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ABSTRACT

This paper presents a numerical model for the estimation of nanocomposite material properties and fracture analysis. A non-uniform peridynamic grid is utilized to simulate the nanocomposites along with Monte Carlo simulation which models single walled carbon nanotube (SWCNT) distribution, dispersion, curvature, orientation, length and diameter. First, a random microstructure is generated from the user inputs consisting of a polymer matrix and SWCNTs. The system is then solved via peridynamic techniques and post-processed to obtain the bulk mechanical properties. Utilizing Monte Carlo simulations, the mean effective modulus for a given set of input parameters is derived. Fracture analysis is performed using a single realization and quasi-static loading conditions via peridynamics allowing simultaneous and spontaneous propagating fractures. The model is validated against experimental data available in the open literature.

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1. Introduction

The role of carbon nanotubes in technology has been rapidly expanding since their discovery in 1952. Carbon nanotubes possess exceptional mechanical, thermal and electrical properties. Experimental studies of single walled carbon nanotubes (SWCNTs) have measured Young's moduli on the order of 1 TPa using direct methods such as with the tip of an atomic force microscope (AFM) [1,2]. These findings have been corroborated using indirect methods which generally includes embedding CNTs in a matrix and loading the composite [3,4]. Further, many theoretical studies have validated this impressive strength [5–8] which is five fold that of steel at one sixth the weight [9]. Experimental studies have also found the electrical conductivity of SWCNTs to be in the range of tens of millions of amps per square millimeter (10^6–10^7A/mm^2) [10,11]. SWCNTs are able to sustain these current densities at high voltages and temperatures without major degradation of the material properties [10] indicating current capacities 1000 times that of copper wire [12]. Thermally, SWCNTs continue to outperform most materials with theoretical thermal conductivities as high as 6000 W/m-K at room temperature [13]. Experimentally, however, thermal conductivities are generally reported to be an order of magnitude lower [14,15] with imperfect bonding and defects being the primary suspect for the difference [16]. These properties make carbon nanotubes exceptional reinforcing agents. These CNT reinforced composites have a multitude of practical applications due to various potential matrix materials and chemical coatings for CNTs. The potential capabilities of nanocomposites and their broad application to many fields has developed a need to reliably predict these material properties and the fracture mechanics of nanocomposites.

1.1. Current models

In the pursuit of a reliable model, many approaches have been reported in the open literature. Frankland et al. [17] and Zhu et al. [18] used molecular dynamics to produce stress–strain curves for SWCNT nanocomposites. These studies reported significant increases in strength for periodic nanotubes. In [19,20] micromechanics models were implemented to model nanocomposites. Effects of waviness and orientation were studied and reported to have a significant effect on the strength of nanocomposites. Multiscale models have also been implemented to great effect. Seidel and Lagoudas [8] developed a two-step process modeling nanotubes as composite cylinders and incorporating them into a continuous matrix using the Mori-Tanka method. Building from this work Spanos and Esteva [21,22] and Spanos et al. [23] developed the embedded fiber finite element method (EFFEM). This model also implements Monte Carlo simulation accounting for stochastic nanotube morphology. However, these models require significant adaptation to model fracture and often require significant

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assumptions to incorporate nanotubes. The proposed model circumvents this by utilizing peridynamics as developed originally by Silling [24] which handles material discontinuities intrinsically. This allows the proposed model to directly incorporate any number of different materials directly without special treatment. Further, peridynamics allows the spontaneous formation and propagation of fracture within a material.

1.2. Peridynamics

The modeling of discontinuities, such as propagating cracks, fracture or material junctions, is a fundamentally challenging part of mechanics and one of ever increasing importance. Peridynamics is a relatively new formulation and falls into the category of non-local mechanics. Non-local mechanics theory was proposed by Kroner and Eringen et al. in the 1960's and 1970's [25,26]. However, Silling developed a new technique called peridynamics which eliminated the need for spatial derivatives [24]. In peridynamics a particle interacts with other distant particles through an integral force which eliminates the need for spatial derivatives and thus allows the modeling of discontinuities without special treatment. In addition, the method allows the spontaneous formation and growth of discontinuities. Peridynamics has been described as a continuum version of molecular mechanics.

Since Silling's original work, many authors have expanded upon the framework of peridynamics. In [27] the method was generalized to a state based model which removed material restrictions from the original method. It was shown in [28] that the one-dimensional peridynamic theory converges to the classical theory as the horizon approaches zero. Peridynamics has also been used to model nanofiber networks including van der Waals forces [29]. In [30] Silling and Askari developed a brittle peridynamic model for use in dynamic simulations. Gerstle et al. [31] used peridynamics to model reinforced concrete structures using MATLAB code. Recently Duzzi et al. [32] applied the peridynamic theory to nanocomposites using several different filler materials. They used a uniform grid and then randomly changed the properties of certain nodes to account for added nanofillers. The authors utilized Silling's original bond-based peridynamic model rather than the state based model.

The bond based model is utilized here as well due to its simplicity. Further, the proposed model incorporates a non-uniform grid through direct placement of nanotube nodes which allows the model to account for nanotube morphology. The nanotube morphology is based upon the work by Spanos and Esteva [21,22] and Spanos et al. [23]. The model also directly incorporates an interface effect between nanotubes and the matrix accounting for material bonding. Further, the proposed model allows for the direct modeling of fracture and crack propagation in nanocomposites which is a difficult but important field of study.

2. Bond based peridynamics

The peridynamic equation of motion is a partial integro-differential equation and describes the motion of a material point at $\boldsymbol{x}$ in the reference configuration at time t and is given as

$$\rho\ddot{\boldsymbol{u}}(\boldsymbol{x}, t) = \int_{\boldsymbol{H}(\boldsymbol{x})} \boldsymbol{f}\left(\boldsymbol{u}\left(\boldsymbol{x}_j, t\right) - \boldsymbol{u}(\boldsymbol{x}, t), \boldsymbol{x}_j - \boldsymbol{x}\right) dV_{\boldsymbol{x}_j} + \boldsymbol{b}(\boldsymbol{x}, t), \tag{1}$$

where ρ is the material density, $\boldsymbol{u}$ is the displacement vector, $\boldsymbol{f}$ denotes the pairwise force function measured in force per unit volume exerted on the point $\boldsymbol{x}$ by the point $\boldsymbol{x}_j$, $\boldsymbol{b}$ is the body force density, and $\boldsymbol{H}(\boldsymbol{x})$ is the domain of point $\boldsymbol{x}$. The relative position in the reference configuration is denoted as

$$\boldsymbol{\xi} = \boldsymbol{x}_j - \boldsymbol{x}, \tag{2}$$

while the relative displacement at time t is

$$\boldsymbol{\eta} = \boldsymbol{u}\left(\boldsymbol{x}_j, t\right) - \boldsymbol{u}(\boldsymbol{x}, t). \tag{3}$$

Therefore, Eq. (1) can be recast as

$$\rho\ddot{\boldsymbol{u}}(\boldsymbol{x}, t) = \int_{\boldsymbol{H}(\boldsymbol{x})} \boldsymbol{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) dV_{\boldsymbol{x}_j} + \boldsymbol{b}(\boldsymbol{x}, t), \tag{4}$$

where $\boldsymbol{H}(\boldsymbol{x})$ is the domain of $\boldsymbol{x}$ defined by

$$\boldsymbol{H}(\boldsymbol{x}) = \left\{\boldsymbol{x}_j : |\boldsymbol{\xi}| \le \delta\right\}. \tag{5}$$

In two dimensions this yields a disk with radius δ centered at $\boldsymbol{x}$. The stretching of bonds in a peridynamic material is given by

$$s(\boldsymbol{\eta}, \boldsymbol{\xi}, t) = \frac{|\boldsymbol{\xi} + \boldsymbol{\eta}| + |\boldsymbol{\xi}|}{|\boldsymbol{\xi}|}. \tag{6}$$

The stretch of the bond is the determining factor as to whether they have failed and hence governs the force between particles similar to strain in classical mechanics theory. Quantifiable damage at a node is given as

$$\phi(\boldsymbol{x}, t) = 1 - \frac{\int_{\boldsymbol{H}(\boldsymbol{x})} \mu(\boldsymbol{\eta}, \boldsymbol{\xi}, t) dV_{\boldsymbol{x}}}{\int_{\boldsymbol{H}(\boldsymbol{x})} dV_{\boldsymbol{x}}}, \tag{7}$$

where total failure of the bond occurs by

$$\mu(\boldsymbol{\eta}, \boldsymbol{\xi}, t) = \begin{cases} 1 \text{ if } s(\boldsymbol{\eta}, \boldsymbol{\xi}, t) < s_0, \\ 0 \quad \text{else}, \end{cases} \tag{8}$$

and s_0 is a predetermined failure criterion.

In linear peridynamics, assuming small displacements, the pairwise force function simplifies to

$$f(\boldsymbol{\eta}, \boldsymbol{\xi}) = \boldsymbol{C}(\boldsymbol{\xi})\boldsymbol{\eta}. \tag{9}$$

The micromodulus tensor is given in [33] as

$$\boldsymbol{C}(\boldsymbol{\xi}) = c_0 \frac{\boldsymbol{\xi} \otimes \boldsymbol{\xi}}{|\boldsymbol{\xi}|^3}, \tag{10}$$

where c_0 is derived from a pairwise micropotential based on a proportional microelastic material model. The peridynamic coefficient, c_0, can be conceptualized as a stiffness coefficient for the bond between two material points and is given for a 2-D plate with a fixed Poisson ratio of $\nu = \frac{1}{3}$ as

$$c_0 = \frac{9E}{h\pi\delta^3}, \tag{11}$$

where E is the Young's Modulus and h is the material thickness. This formulation is derived from equating the strain energy of a peridynamic material to that of a regular continuum material [31,34,35].

2.1. Discretization

The static load being applied to a single point volume, $\boldsymbol{x}_i$, by every other point within its horizon, $\boldsymbol{x}_j$, is given by

$$0 = \int_{\boldsymbol{H}_i} \boldsymbol{C}(\boldsymbol{\xi})\boldsymbol{\eta} dV_{\boldsymbol{x}_j} + \boldsymbol{b}_i. \tag{12}$$

Discretizing the right hand side of Eq. (28) and expanding $\boldsymbol{\eta}$ yields

$$0 = \sum_{j}^{N} \boldsymbol{C}(\boldsymbol{\xi})(\boldsymbol{u}_j - \boldsymbol{u}_i) V_j + \boldsymbol{b}_i. \tag{13}$$

This can formed into a stiffness density matrix where the 2×2