MUTLISCALE MODELING OF THE INELASTIC BEHAVIOR OF THE NANO-REINFORCED COMPOSITES

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Introduction

Nanoscale materials may find use in a wide range of applications in defense, automotive and medical industries, such as material reinforcement, nanoelectronics, chemical sensing, medical diagnostic, and drug delivery. In particular, materials such as carbon nanotubes, nanotube and nano particle-reinforced composite materials have shown considerable promise compared to typical carbon fiber reinforced composites.
In order to facilitate the development of nanoscale materials the field needs a development of a rational and reliable model that accurately bridges the scale up issues from the nanoscale to the macroscale.
Few methods have been proposed for the modeling the mechanical behavior of the single walled carbon nanotube(SWCN) and multi walled carbon nanotube (MWCN) reinforced composite. Odegard et al.[1] developed an equivalent continuum modeling approach for the SWCN polymer composites. Alternatively molecular structure mechanics approach is proposed by Li and Chou [2] to evaluate elastic mechanical properties of the carbon nanotube reinforced composite materials.
In this paper multi scale constitutive relationships are developed to predict the inelastic response of the carbon nanotube reinforced composite as a function of the molecular structure of its constituents.

Multiscale modeling approach.

Equivalent Continuum Modeling

The equivalent continuum modeling method developed by Odegard et al. [1] is used here The major steps of this model are follows(i) establishing representative volume elements (RVEs) for molecular and equivalent continuum models (ii) the potential energies of deformation for the molecular model and effective fiber were derived and equated for identical loading conditions in order to obtain elastic properties of the nanotube fiber in terms of the force constants of the molecular systems (iii) the overall constitutive properties of the dilute unidirectional SWCNT reinforced composite were determined with the micromechanical based models.

Molecular dynamic potential

The bonded and non-bonded interactions of the atoms in a molecular structure can be quantitatively described by using molecular mechanics. The force that exists for each bond as a result of the relative atomic positions is described by the force field such that these forces contribute to the total molecular potential energy of a molecular system. One of the functional forms of these potentials depending on the particular material and loading conditions is given as

$$U^{MD} = \sum K_a^{\rho}\left(\rho_a - P_a\right)^2 + \sum K_a^{\theta}\left(\theta_a - \Theta_a\right)^2 \qquad (1)$$

where the terms P_a and Θ_a refer to the undeformed interatomic distance of bond umber "a" and the undeformed bond angle number "a", respectively. The quantities ρ_a and θ_a are the distance and bond angle after stretching and angle variance, respectively. The terms K_a^{ρ} and K_a^{θ}

represent the force constants associated with the stretching and angle variance of bond and bond angle number "a" respectively.

Equivalent truss model

In order to express the mechanical strain energy, U^{Truss} of the truss model in terms of the variable truss joint angles that are specified in the molecular model, the RVE is modeled with additional rods between nearly adjacent joints to represent the interaction between the corresponding carbon atoms. The mechanical strain energy, U^{Truss} of the discrete truss system is then calculated.

Equivalent continuum for the effective fiber

The geometry of linear elastic homogeneous, equivalent continuum RVE was assumed to be cylindrical, similar to that of the molecular and truss models. Within this approach the mechanical properties of the solid cylinder were determined by equating the total strain energies of the equivalent truss and equivalent continuum models under identical loading conditions. The generalized total elastic strain energy of the effective fiber is given as

$$U^{Fiber} = \frac{V}{2}\sigma_{ij}\varepsilon_{ij} = \frac{\pi D^2 L}{8}\sigma_{ij}\varepsilon_{ij} \qquad (2)$$

where D is the diameter, L is the length and V is the volume of the effective fiber.

Modeling of two phase composite material

The effective fiber having different orientation accurately accounts for the structure-property relationship at the nanoscale. It also provides a bridge to continuum models that may be developed within a micromechanical frame by using the mechanical properties of the effective fiber and plastic matrix.

Analysis and results

The proposed multiscale theoretical model is used here to calculate the effective elastic modulus for the polymer composite material which is made of LaRC-SI, a thermoplastic ploymide and single walled carbon nanotube. The results are presented in Figure 1

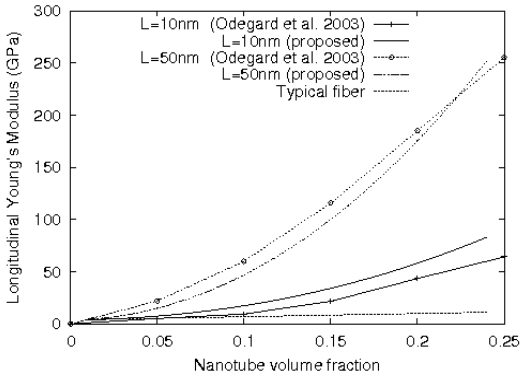

Fig. 1: Longitudianal Young's modulus of polymer composite vs. nanotube volume fraction.

The Young's modulus of the aligned effective fiber is plotted in this figure with respect to volume fraction of nanotube that are 10 and 50nm long. The results of the proposed model are compared with that of Odegrad et al 's model. The both show same trend in their predictions of Young's modulus where it increases with an increase in volume fraction.

Conclusion

A multiscale frame work for the constitutive models for carbon nanotube reinforced composite material is presented. The equivalent continuum nanotube is then assumed to be dispersed inside matrix material where its behavior is modeled as the gradient dependent theory plasticity [3]. Finally the overall response of the nanotube reinforced composite is obtained by using average mean field approaches such as the Mori Tanaka averaging scheme.

References

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