MULTIFUNCTIONAL NANO-TAILORED COMPOSITES FOR IN SITU SELF-HEALTH MONITORING OF AIRCRAFT STRUCTURES

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Summary In this research, we intend to introduce multifunctionality into epoxy adhesives through the homogeneous dispersion of carbon nanotubes (CNTs). Specifically, we are interested in improving the mechanical properties and electrical conductivity of the adhesive. The increased electrical conductivity would facilitate the use of the embedded nanofillers for sensing *in situ local damage*, thus allowing the quantitative in-flight self-health monitoring of structural adhesive bonds (SABs).

INTRODUCTION

The outstanding mechanical and electrical properties of CNTs make them ideal candidates for use as reinforcing agents in polymer materials. However, excellent intrinsic nanotube properties do not necessarily translate into the same properties for the bulk composite. Several issues pertaining to the alignment, dispersion, aspect ratio, orientation and load transfer need to be optimized in order to achieve the best properties of the composite. Since experimentation at the nanoscale is still a developing field, the best way to quantify the effects of such parameters is through computational modeling techniques. Here we adopt the atomistic-based continuum (ABC) multiscale modeling technique to predict the mechanical properties of the composite system. It has the unique advantage of describing atomic positions, their interactions and their governing interatomic potentials in a continuum framework. Thus, the influence of the nanophase is taken into account via appropriate atomistic constitutive formulations. Consequently, these measures are fundamentally different from those in the classical continuum theory. The strength of ABC techniques lies in their ability to avoid the large number of degrees of freedom encountered in the concurrent techniques, whilst at the same time allow for the description of the nonlinear constitutive behaviour of the constituents.

Any model which attempts to characterize the electrical conductivity of a composite system containing CNTs must account for three fundamental contributions; the intrinsic resistance of the CNTs, the tunneling resistance between neighboring CNTs, and the contact resistance at CNT junctions. The electrical conductivity of the composite system is predicted using a combination of Monte Carlo and equivalent resistor network models whereby each of these contributions are modeled as an individual resistor in an electrical circuit representative of the composite system. A schematic of this approach is depicted in Fig. 1.

ATOMISTIC-BASED CONTINUUM MODEL

A three-dimensional nonlinear representative volume element (RVE) was developed to study the nano-reinforced polymer system. The RVE consists of the carbon nanotube (CNT), the surrounding polymer matrix, and the CNT-polymer interface. The CNT was modeled as a space-frame structure as depicted in Fig. 2. In the space-frame model, each beam element corresponds to an individual chemical bond in the CNT. As in traditional FE models, nodes were used to connect the beam elements to form the CNT structure. In this case the nodes represent the carbon atoms and their positions are defined by the same atomic coordinates. In this way, the space-frame structure allows the mechanical behavior of the CNT to be accurately modeled in terms of the displacements of the atoms.

Figure 2 also illustrates a portion of the hexagonal lattice to demonstrate the connectivity of the beam elements in the continuum representation of the CNT. The Modified Morse interatomic potential was used to derive the material models for the continuum representations of the atomic interactions in the CNT. This potential accurately accounts for both bond stretching and bond bending deformation mechanisms and its general form is given as;

$$E = D_e \left[1-\exp^{-\beta\, r-ro}\right]^2 -1 + \frac{1}{2}k_\theta \left(\theta-\theta_o\right)^2\left[1+k_{sextic}\left(\theta-\theta_o\right)^4\right] \tag{1}$$

The surrounding adhesive was modeled as a homogeneous solid with properties representative of typical aerospace epoxies. The volume of the polymer was varied in order to investigate the effect of the CNT's volume fraction on the effective mechanical properties of the nano-reinforced polymer system.

In this study, we investigate a non-bonded configuration which implies that only van der Waals interactions are considered. In order to simulate the van der Waals interactions, we have adopted the use of a truss rod model whereby each interaction was represented by one truss rod. Each rod extends out from a carbon atom in the CNT structure to an atom in the polymer matrix. The Lennard-Jones potential was used to describe the behavior of the van der Waals interactions. For further details regarding this model the reader is referred to Ref. [1]

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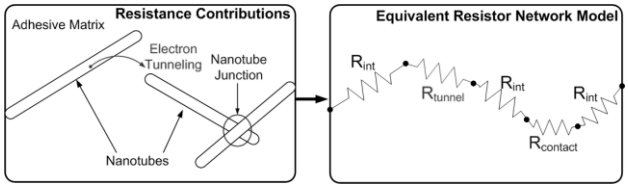

Fig. 1: Equivalent resistor network model.

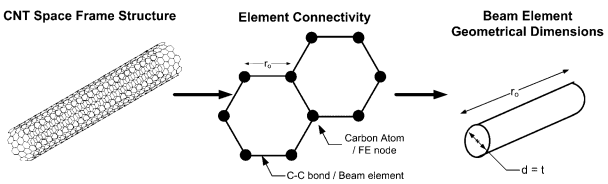

Fig. 2: Carbon nanotube space frame structure.

EQUIVALENT RESISTOR NETWORK MODEL

The intrinsic electrical resistance of the CNTs is evaluated using a constitutive law based on the Drude model which assumes a constant electrical conductivity along the CNT. The resistance is given by:

$$R_{\text{int}} = 4l / \pi \sigma D^2 \tag{2}$$

The tunneling and contact resistance are evaluated using the Laundauer-Buttiker formula which accurately describes the ballistic electron transport between neighbouring CNTs. The formula contains the transmission probability T which is a function of the separation distance. As the distance reaches its minimum the formula reduces to the contact resistance. The Laundauer-Buttiker formula is given by;

$$R_{\text{int}} = h / 2e^2 MT \tag{3}$$

RESULTS AND DISCUSSION

As an intermediate step in the study of the effective mechanical properties of nano-reinforced composites, the nonlinear response of individual CNTs were investigated. Figure 3 shows the predicted stress-strain curves for armchair and zigzag nanotubes. The results show that the zigzag nanotube can withstand a strain of 17%, while the armchair nanotube can withstand a strain of up to 22%. The respective tensile modulus for the armchair and zigzag nanotubes are 944.8 GPa and 920.2 GPa. The overall trend of the stress-strain curves agree well with others in the literature.

Figure 4 shows the predicted electrical conductivity of the nanocomposite for varied CNT concentrations and intrinsic conductivities. From these predictions we can extrapolate a percolation threshold of approximately 0.1 vol%. The significance of these results lies in the ability to introduce electrically conductive capabilities to the resulting composite through the dispersion of very low concentrations of CNTs.

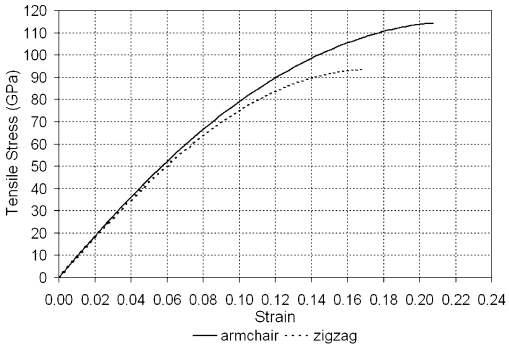

Fig. 3: Nanotube stress-strain curves.

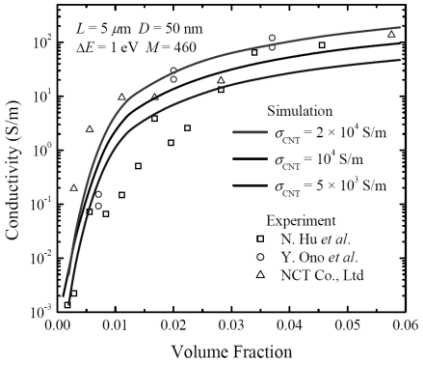

Fig. 4: Electrical conductivity of resulting composite.

FUTURE WORK

As an extension of the current numerical work micromechanical models will be developed to extend the results to the macroscopic scale. In addition, the electrical footprint of common damage phenomena will be investigated. Here the ABC and resistor network models will integrated into a unified model. In this way we hope to demonstrate the potential to use CNTs networks as sensors of *in situ local damage* of structural adhesive bonds.

References

[1] Wernik J.M., Meguid S.A., Acta Mechanica **217**: 1-16, 2011.