A Functionally Graded Multi-Phase Micromechanical Model for Carbon Nanotube – Polymer Composites

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Introduction

Carbon nanotubes (CNT) have some outstanding properties in the mechanical, electrical and electronics, and thermal domains. Their stiffness and strength are some of the greatest ever observed. The stiffness and strength of sample carbon nanotubes are compared to those of some widely used engineering materials in Figure 1.

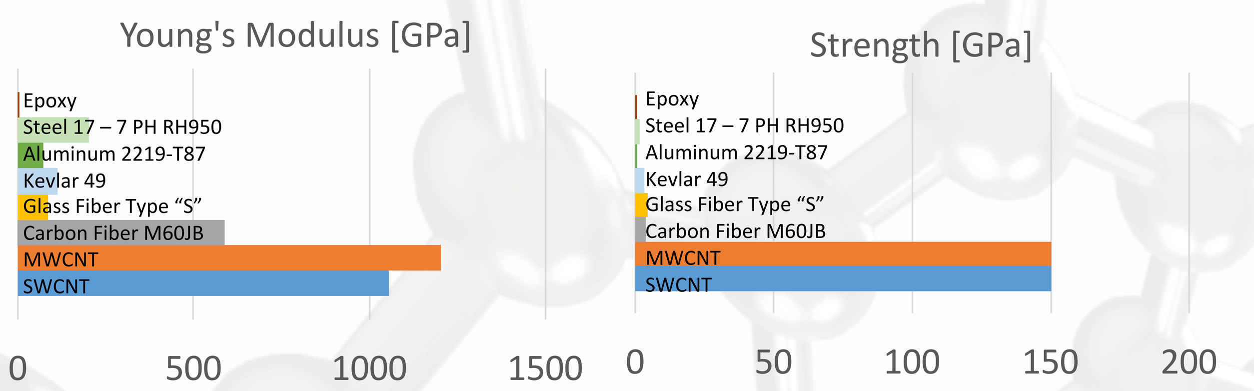

Figure 1: Stiffness and strength of Single Walled Carbon Nanotubes (SWCNT) and Multi-Walled Carbon Nanotubes (MWCNT) compared to some engineering materials.

Micromechanics offers a very easy to use and simple, yet strong methods for analyzing nano composites. The vast majority of currently used micromechanical models use 2 or 3 phases to represent a CNT nanocomposite. Recently published observations suggest that there are at least 4 distinct phases in a carbon nanotube composite; the CNT the interface (IF), the interphase (IP), and the polymer (Pol). Furthermore the density distribution of the interphase suggests that it can be better modelled using a functionally graded micromechanical phase [2]. In this paper we use a multi-inclusion micromechanical model to simulate a carbon nanotube – polymer composite in which the interphase is modelled in a functionally graded manner and the combination of the interface and the CNT is replaced by an effective fiber characterized by finite element modeling.

Abstract

In this study we employ a multi-inclusion micromechanical model to analyze carbon nanotube – polymer nanocomposites. The nanocomposite was divided into four phases consisting of the carbon nanotube, the interface, the interphase and the bulk polymer. The combination of the carbon nanotube and the interface was transformed into an effective fiber using Finite Element (FE) modeling. The interphase was graded in a functional manner. The results of the analyses were compared to other experimental and numerical studies in the literature.

Acknowledgements

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Phase Properties

The elastic moduli of the carbon nanotubes and the interface were obtained from [4]. The CNTs have transversely isotropic properties while the interface was assumed to be isotropic. The interface is assumed to be 3.4 Å thick. The interface and the CNT were then combined into a single effective fiber through FE by matching displacement under various loading conditions described in Figs. 3-6. The loads include uniform axial pressure, uniform lateral pressure and uniform axial torsion.

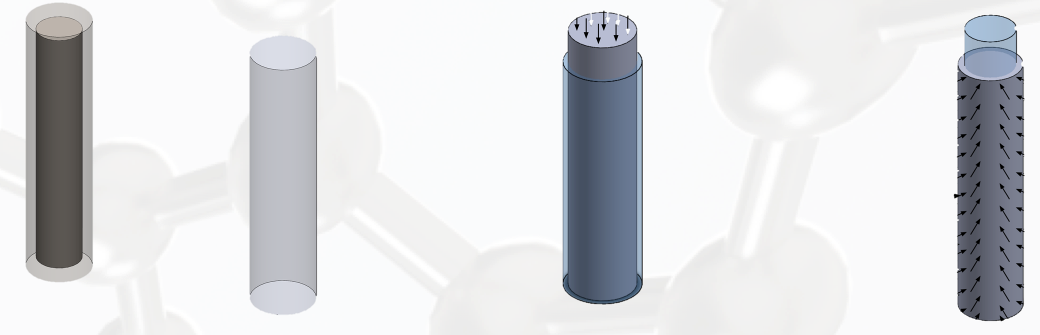


Figure 3: Cut sections of the finite element models consisting of CNT and the interface (left), and effective fiber (right).

Figure 4: Loading conditions used to obtain the longitudinal modulus of the effective fiber.

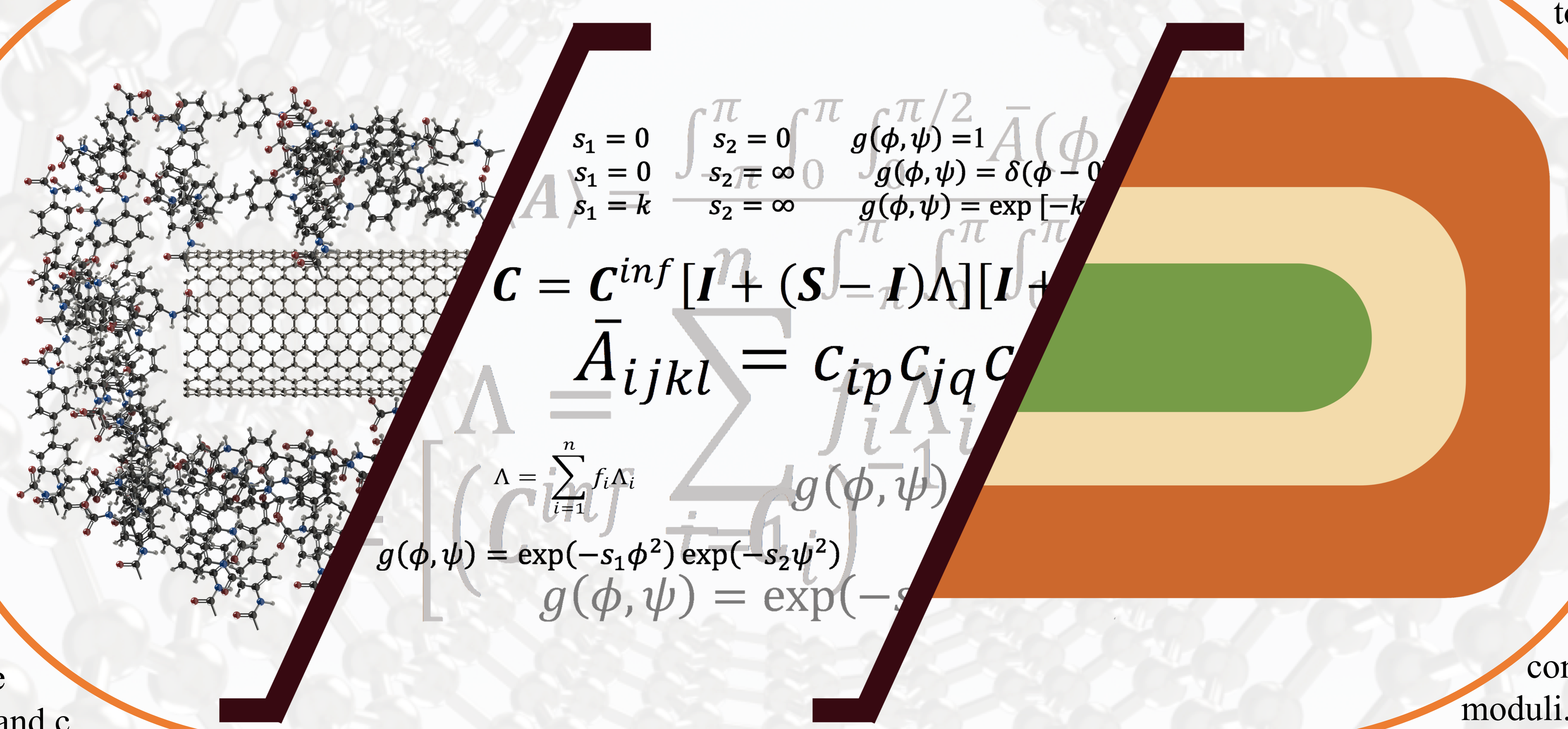
Figure 5: Loading conditions used to obtain the transverse modulus and Poisson's ratio ν_{12} of the effective fiber.

CNT Radius	E_1	E_2	G_{12}	ν_{12}	ν_{23}
[Å]	[GPa]	[GPa]	[GPa]	[-]	[-]
3.9	113.0	38.0	40.0	0.32	0.2
5.5	112.0	19.6	49.0	0.32	0.2
7.1	73.2	17.0	39.0	0.34	0.2

Table 3: Elastic moduli of the effective fiber

Figure 6: Loading conditions used to obtain G_{12}.

The elastic moduli of the interphase were assumed to vary from the effective fiber to the polymer in a linear or exponential manner or stay constant. The polymer is modelled after LARC-SI and has a Young's modulus of 3.8 GPa and a Poisson's ratio of 0.4



Methodology

The micromechanical model used in this study is adopted from [3]. The phases of the model are assumed to be perfectly elastic, coaxial and similar in shape such that $a_1/a_2 = b_1/b_2 = c_1/c_2 = \gamma$ where a, b and c are the physical dimensions of the inclusions as seen in Figure 2. The elastic moduli, $\boldsymbol{C}$, of the composite consisting of n phases is given in (1) where $\boldsymbol{I}$ is the 4[th] order identity tensor, $\boldsymbol{S}$ is the Eshelby tensor [4], $\boldsymbol{C}^{inf}$ is the moduli tensor of a fictitious infinite domain. The infinite domain characterizes the resulting composite material and hence the moduli were iteratively modified until they matched those of the resulting nanocomposite.

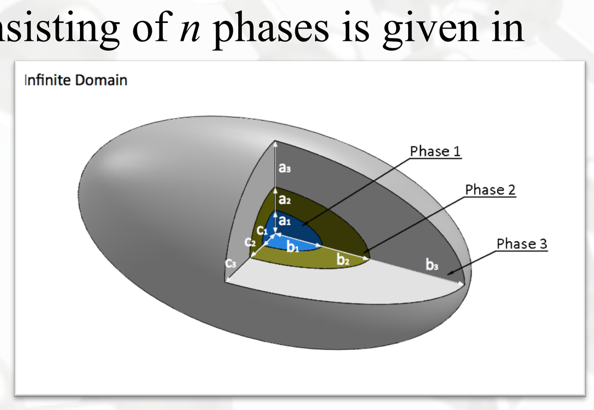


Figure 1: Figurative representation of the micromechanical model.

$$\boldsymbol{C} = \boldsymbol{C}^{inf}[\boldsymbol{I} + (\boldsymbol{S} - \boldsymbol{I})\Lambda][\boldsymbol{I} + \boldsymbol{S}\Lambda]^{-1} \quad (1)$$

$$\Lambda = \sum_{i=1}^{n} f_i \Lambda_i$$

$$\Lambda_i = \left[(\boldsymbol{C}^{inf} - \boldsymbol{C}_i)^{-1}\boldsymbol{C}^{inf} - \boldsymbol{S}\right]^{-1} \quad (2)$$

$$\Lambda_i = \frac{3}{1-\gamma^3}\int_\gamma^1 r^2 \lambda_i(r)dr \quad (3)$$

$$\lambda_i = \left[(\boldsymbol{C}^{inf} - \boldsymbol{C}_i(r))^{-1}\boldsymbol{C}^{inf} - \boldsymbol{S}\right]^{-1}$$

$$\langle \boldsymbol{A} \rangle = \frac{\int_{-\pi}^{\pi}\int_0^{\pi}\int_0^{\frac{\pi}{2}} \bar{A}(\phi,\gamma,\psi)\, g(\phi,\psi)\sin(\gamma)\, d\phi\, d\gamma\, d\psi}{\int_{-\pi}^{\pi}\int_0^{\pi}\int_0^{\frac{\pi}{2}} g(\phi,\psi)\sin(\gamma)\, d\phi\, d\gamma\, d\psi} \quad (5)$$

$$\bar{A}_{ijkl} = c_{ip}c_{jq}c_{kr}c_{ls}A_{pqrs}$$

$$g(\phi,\psi) = \exp(-s_1\phi^2)\exp(-s_2\psi^2) \quad (6)$$

Here the definition of Λ depends on whether a given inclusion is functionally graded or not. For inclusions of constant mechanical properties Λ is given in (2) while in inclusions where the mechanical properties are variable the parameter Λ is calculated as in (3) The orientation averaging integral of a tensor A is denoted as $\langle \boldsymbol{A} \rangle$ and is defined in (5) where c_{ij} are the direction cosines for the transformation and g is the orientation distribution function defined in (6). s_1 and s_2 are parameters that control the orientation.

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Results and Discussion

The interphase can be modelled using a constant, linear and exponential distribution of moduli. Figure 6 plots modulus enhancement with respect to polymer for various CNT radii and interphase moduli distribution. It can be seen that constant and linear distributions generate unreasonably high reinforcements. Hence an exponential distribution is seen as more appropriate. In Figure 8 we compared some results found in the literature with ours for various interphase thicknesses and CNT radii. The plots suggest that an interphase thickness of 10 Å more closely simulates the nanotube than the alternatives. Last but not least a study of the effect of aspect ratio on the composite moduli was performed as seen in Figure 7. A lower aspect ratio means the nanotube has less contact area for adhesion with the polymer. As such lower aspect ratios have resulted in decreased nanotube performance. However moduli seem to have stabilized at around 50.

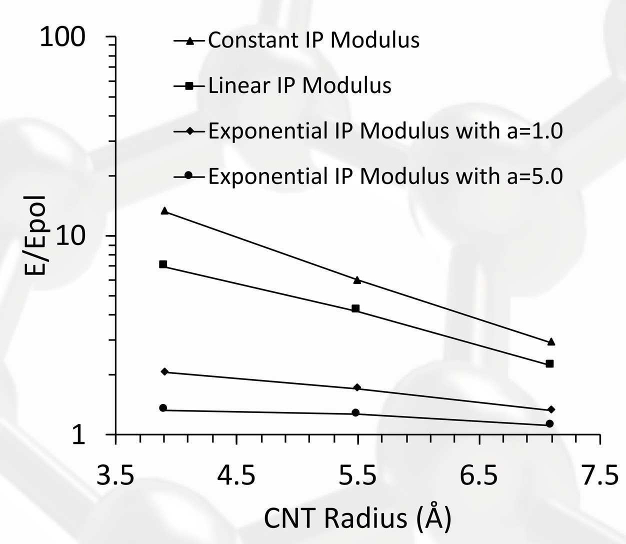

Figure 6: Young's modulus of nanocomposite with %1 vol. effective fiber normalized by that of the polymer vs CNT radius using various functions for interphase modulus distribution.

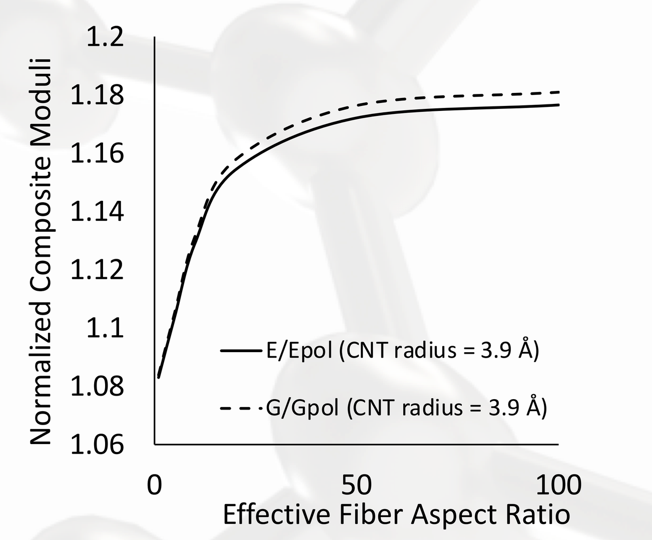

Figure 7: Composite Young's and shear moduli vs effective fiber aspect ratio.

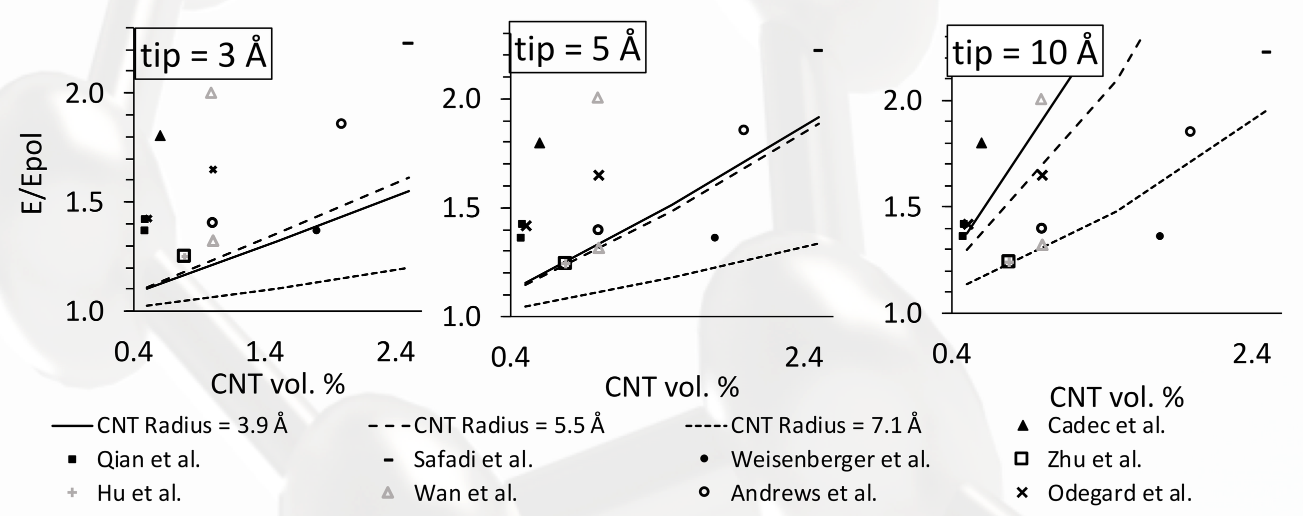

Figure 8: Improvement in polymer Young's modulus vs CNT vol.% for various CNT radii and interphase thicknesses, t_{ip}, for a = 1.