Evaluation of effective properties for smart graphene reinforced nanocomposite materials

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ABSTRACT

In this study, analytical and numerical models were developed to investigate the effective properties of graphene reinforced nanocomposite (GRNC) subjected to electromechanical loading. In this analytical mechanics of material (MOM) model was developed to predict effective properties of the composite while numerical finite element (FE) model developed with the help of a representative volume element (RVE). Also, the longitudinal and transverse modulus of GRNC is determined using the Halpin-Tsai equations. Both models are showing a good agreement for loading applied along the fiber direction when compared to transverse loading. The present study highlights on developing efficient NEMS application.

1. Introduction

A composite material is the combination of two or more constituents, combined at a macroscopic level and are insoluble in each other. One constituent is called the reinforcing phase and the another one in which it is incorporated is called the matrix. The piezoelectric material has a superior characteristic such that coupling between the mechanical and electrical effect. Due to this piezoelectric material is specifically used in the application of smart sensors, transducers, and actuators. To meet increasing demands polymer matrix composite for structural strength and energy efficiency, carbon nanotube (CNT) reinforced polymer composites have been examined thoroughly over the past few decades. The main challenge lies in attainment of CNTs that uniformly dispersion and CNT give exceptional mechanical properties only when integrated with very small concentrations. Hence, a composite made of graphene and its derivatives with polymer is an auspicious material for many engineering applications due to its lightweight and comparatively high strength properties. Graphene is considered to be one of the rising star of the horizon in materials of the twenty-first century. It is a highly emerging candidate of materials science and conceptually relativistic. Astonishingly, high mobility of electron as well as its striking features, such as abnormal pseudo-magnetic field, spin transport, and quantum Hall effect. Graphene is a 2-D covalently bonded network of carbon atoms. It has numerous interesting properties such as electro-thermo-mechanical, optical, and magnetic etc. Graphene is used in different application such as ion-lithium batteries, transistors, electrodes, and sensors. Reuss outlined several micromechanical models established to calculate the macroscopic behavior of polymeric composite materials reinforced with typical reinforcements such as carbon or glass fibers. These micromechanical models were based on assumption that the fiber, matrix, and sometimes the interface are continuous materials and the constitutive equations for the bulk composite material are expressed based on assumptions of continuum mechanics. Numerous micromechanical models have been established by researchers to envisage the effective properties of composites with different methods.

The aim and objective of this work are to estimate effective elastic and piezoelectric properties of the GRNC. In this work, the FEM-based numerical analysis is conceded using commercial software ANSYS-15.0 while the analytical calculation is carried out using the MOM model.
2. Modeling

2.1. Micromechanical model

The major objective of micromechanical model is to estimate the effective overall properties in terms of the properties of the constituents and their microstructure. Assuming that the graphene as solid fiber, the micromechanical model developed by Kundalwal and Ray [11] to govern the effective properties of an elastic coefficient \( [C^{nc}] \) of the polymer matrix nanocomposite (PMNC). Based on this, the effective elastic, as well as piezoelectric properties of GRNC, are derived.

The relation between the stress and strain of respective phases of proposed GRNC can be written in the following form,

\[
\sigma^r = [C^r]_{6 \times 6} \varepsilon^r, \quad r = f, m, \text{ and } nc
\]  

(1)

where \( \sigma^r \) denotes the stresses, \( \varepsilon^r \) the strains, and \( C^r \) the elastic constant of a matrix of the \( r \)th phase. The superscripts \( f, m, \) and \( nc \) used in Eqs. (1) are for corresponding graphene fiber, matrix, and the nanocomposite respectively. Using the rules of the mixture and iso-field condition bond between the reinforced graphene and polyimide matrix is considered to be perfect and it can be written as

\[
\{\sigma^f\} = \{\sigma^{nc}\} = \{\sigma^m\}
\]

(2)

\[
\nu^r \{\sigma^f\} + \nu^m \{\sigma^m\} = \{\sigma^{nc}\}
\]

(3)

In Eq. (3), \( \nu^r \) and \( \nu^m \) are respective volume fraction of the graphene fiber and polyimide matrix. By correlating the Eqs. (1)–(3) stresses and strains can be written as follows:

\[
\{\sigma^{nc}\} = [C_1] \{\varepsilon^f\} + [C_2] \{\varepsilon^m\}
\]

(4)

\[
\{\varepsilon^{nc}\} = [V_1] \{\varepsilon^f\}_{6 \times 1} + [V_2] \{\varepsilon^m\}_{6 \times 1}
\]

(5)

Also, using Eq. (2) we can write

\[
[C_1] \{\varepsilon^f\} - [C_4] \{\varepsilon^m\} = 0
\]

(6)

The matrix \( [C^{nc}] \) in Eq. (7) gives the effective elastic properties of the GRNC material.

\[
[C^{nc}] = [C_1][V_1]^{-4} + [C_2][V_2]^{-4}
\]

(7)

\[
[V_1] = [V_1][C_4]^{-1}[C_1]; [V_2] = [V_2][C_4]^{-1}[C_2]
\]

(8)

here, matrices from \( C_1-C_4 \) and \( V_1-V_4 \) obtained using some assumptions and curtailments. To obtain the elastic modulus, shear modulus, and Poisson’s ratio we have the expression as follows:
where $\eta = \left(\frac{\varepsilon_f}{\varepsilon_m}\right)^{-1}$

In the above equation, $\xi$ is used to denote the reinforcing factor and it depends on the fiber geometry, packing geometry and loading conditions. For example, $\xi = 2$ for circular fibers in a packing geometry of a square array while width b in a hexagonal array along the loading direction, for a rectangular fiber $\xi = 2(a/b)$.

Major poisson ratio ($\nu_{12}$) : $\nu_{12} = \nu_{ij}^{\varepsilon} + \nu_{ij}^{E}$

(15)

In-plane shear modulus ($G_{12}$) : $G_{12} = \frac{C_{12}}{C_{m}} = \frac{1 + \eta \nu_{ij}^{E}}{1 - \eta \nu_{ij}^{\varepsilon}}$

(16)

where $\eta = \left(\frac{\varepsilon_f}{\varepsilon_m} + 1\right)/\left(\frac{\varepsilon_f}{\varepsilon_m} - 1\right)$

In this case, $\xi = 1$ for circular fibers in a square array, $\xi = \sqrt{3} \log_2(a/b)$, where $a$ is the direction of loading.

2.2. Finite element modeling

In this section, the modeling of the finite element (FE) is proposed with the help of commercial ANSYS 15.0 package to compare the results derived from the MOM model for effective piezoelectric properties. The FE model for piezoelectric composite is developed by various authors [13–15]. This analysis is fully coupled electromechanical analysis in which modeling of 3-D representative volume element is made with 20 node brick elements solid 226 having both displacement and voltage degree of freedom. From Fig. 1, RVE of GRNC is analyzed under the homogenization of composite by incorporating various boundary conditions. Hence, the total average value of homogenized laminate is obtained using equation are as follows:

\[
\bar{\sigma}_{ij} = \frac{1}{V} \int \sigma_{ij} dV; \quad \bar{\tau}_{ij} = \frac{1}{V} \int \tau_{ij} dV; \quad \bar{E}_i = \frac{1}{V} \int E_i dV; \quad \bar{D}_i = \frac{1}{V} \int D_i dV \tag{17}
\]

\[
\begin{bmatrix}
\bar{\sigma}_{ij} \\
\bar{\tau}_{ij} \\
\bar{E}_i \\
\bar{D}_i
\end{bmatrix} = \begin{bmatrix}
C_{ij}^{\varepsilon} & -e_{ij}^{\varepsilon} \\
e_{ij}^{\varepsilon} & K_{ij}^{\varepsilon}
\end{bmatrix} \begin{bmatrix}
\bar{\varepsilon}_{ij} \\
\bar{E}_i
\end{bmatrix}
\tag{18}
\]

where $\sigma_{ij}$ are the stresses; $\tau_{ij}$ are the shear stresses; $\varepsilon_{ij}$ are the strains; $E_i$ are the electrical field; and $x_{ij}$ are the components of dielectric constants.

2.2.1. Effective elastic coefficient $C_{23}^{\varepsilon}$ and $C_{33}^{\varepsilon}$

For the estimation of effective elastic coefficients $C_{23}^{\varepsilon}$ and $C_{33}^{\varepsilon}$, the boundary condition can be imposed uniform displacement to RVE (shown in Fig. 2) in such a way that besides the surface of RVE in the z-direction, all other surfaces in x and y-directions must be constrained in its normal direction. Due to the boundary condition, only normal strain in z-direction i.e., $\bar{s}_{33}$ should be present in the unit cell ($s_{11} = s_{22} = s_{23} = s_{13} = s_{12} = 0$). In the same way, the electric field ($E_1 = E_2 = E_3 = 0$) at all faces should be constrained to zero. From Eq. (17), average stress in y and z-direction ($\bar{s}_{23}, \bar{s}_{33}$) and average strain in the z-direction ($\bar{e}_{33}$) can be obtained. Then using Eq. (18), $C_{23}^{\varepsilon}$ and $C_{33}^{\varepsilon}$ can be calculated as the ratio of $s_{33}/e_{33}$ and $s_{23}/e_{33}$, respectively. For the sake of brevity, we have not explained the detailed FE procedure for remaining coefficient and reader are referred to [15] for a more comprehensive detail. Similarly, all the remaining effective coefficients $C_{11}^{\varepsilon}$, $C_{12}^{\varepsilon}$, $C_{44}^{\varepsilon}$, $C_{66}^{\varepsilon}$, $e_{23}^{\varepsilon}$, and $e_{33}^{\varepsilon}$ can be determined using suitable boundary conditions to RVE.

3. Result and discussion

In this section, the numerical values are evaluated in the earlier section using the two different methods such as micromechanical model (MOM) and finite element (FE) method for the GRNC. The corresponding elastic, piezoelectric, and dielectric properties of pristine graphene fiber and polyimide matrix are shown in Table 1.

In order to check the results from this study, the effective elastic coefficient and piezoelectric properties of GRNC material derived using both MOM and FE model shows good coherence for the different volume fraction of graphene ranges from 0.2 to 0.7. From this it can be determined that Fig. 3 shows the effective properties against the fiber volume fraction of graphene fiber. It is clearly seen that the effective elastic, and piezoelectric constants ($E_3$ and $e_{33}$) showing indistinguishable results. Such estimations clearly fit with the Voigt-upper bound and linearity. In case of $E_1$ and $G_{12}$ the
results for FEM model overestimates the MOM model estimations [12,14]. It is due to the fact that these coefficients are matrix dependent and influenced by in-plane behavior of composite. Hence, it is important to mention that piezoelectric composite material shows good coherence when loading is applied in the axial direction as compared to loading applied in the transverse direction. It can be concluded from comparisons shown in Fig. 3 that the numerical results obtained by the MOM and FE models are in excellent agreement[12,14] while the results for the remaining effective constants such as $G_{13}, G_{23}, \nu_{13},$ and $\nu_{12}$ are obtained from the Halpin Tsai formulations but not shown here for the sake of brevity.

### 4. Conclusion

In current study, the micromechanical model (MOM) is developed for the derivation of effective properties of graphene reinforced nanocomposite materials and these properties are compared with finite element (FE) model for different volume fraction. From this study, it can be observed that if the loading is applied along the axial direction then the effective axial modulus shows the linearity for both models. From this it is clear that there is relation between Young’s modulus and effective elastic i.e., stiffness coefficients. The effective stiffness coefficients depend on the Poisson’s ratio. Also, the transverse modulus shows good results with Halpin Tsai formulations. While curves of the transverse and shear effective properties show a marginal difference from the analytical and numerical FE model mainly because they are influenced by in-plane behavior and large constrain imposed to RVE of GRNC. Hence proposed GRNC may become most convincing materials for use in evolving efficient smart structures such as sensors and actuators in NEMS application.

### Acknowledgements

The authors gratefully acknowledge the financial support provided by the Indian Institute of Technology Indore and the Science Engineering Research Board (SERB), Department of Science and Technology, Government of India. S.I.K. acknowledges the generous support of the SERB Early Career Research Award Grant (ECR/2017/001863).

### References


