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DETERMINATION OF ELASTIC CONSTANTS OF HYBRID COMPOSITES BY A TWO-STEP COMPUTATIONAL HOMOGENIZATION APPROACH

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ABSTRACT

The work aims to study hybrid composites in which carbon nanotubes are grafted radially on a carbon fiber surface in a polymer matrix. One of the challenging topics in hybrid composites is characterization. The effective properties of this material, fuzzy fiber composites (FFC), are computed via computational homogenization methods. At first, a micromechanical method is followed to obtain the mechanical properties of the graded interphase region. FEM analyses are conducted after obtaining the interphase's homogenized properties. Finally, a subroutine in MATLAB is written to calculate the homogenized properties of the FFC using the finite element results.

INTRODUCTION

A composite material is a kind of material that consists of at least two different constituents, generally an inclusion and a matrix. With this constitution, it becomes very functional due to its superior properties such as lightweight, higher strength, high impact resistance, and resistance to fatigue and corrosion. Moreover, composite materials can be tailored according to where they will be used, giving them a huge utilization area. Thus, they are widely used in many sectors, such as aerospace, civil, medical engineering, etc.

Since the discovery of carbon fibers, carbon-reinforced polymer composites, which consist of carbon as an inclusion and a polymer matrix, have gained importance for their structural performance. However, despite the successful structural performance of these materials, the poor mechanical properties of the fiber-matrix interface restrict the novel properties of the composites. To improve the mechanical properties of the fiber-matrix interface, the most common technique is to introduce a third phase between the fiber and matrix, named interphase, as shown in Figure 1. As interphase, carbon nanotubes can improve the interfacial adhesion properties and increase the fiber's surface area [Kim et al., 2015].

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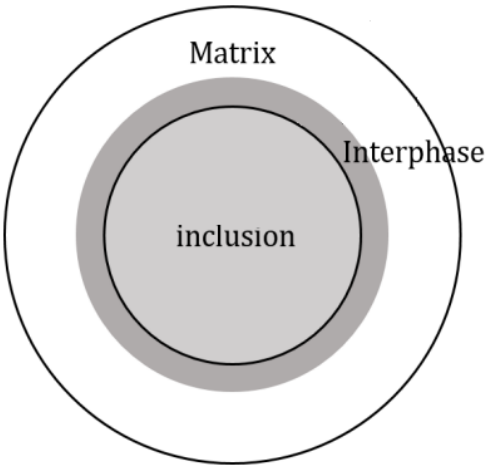


Figure 1: Introduction of interphase as a third phase around the inclusion.

In recent years, fuzzy fiber composites (FFC) have also gained importance with the discovery of superior mechanical and electrical properties of carbon nanotubes (CNT). A fuzzy fiber composite is a material that inclusion is carbon fiber, and around the fiber, there are radially grown CNTs (forest of carbon nanotubes) on the fiber, as shown in Figure 2. In the literature, plenty of experiments have already validated the properties of FFCs, such as flexural elastic modulus, inter-laminar shear strength, fracture toughness, etc. In the study of [Cheng et al., 2019], FFC is compared with traditional fiber-reinforced composites. This study showed that the transverse modulus increases by 30-50%, and the shear modulus increases by more than 20%. The tensile modulus is almost unaffected; the change in tensile modulus is less than 1.5%.

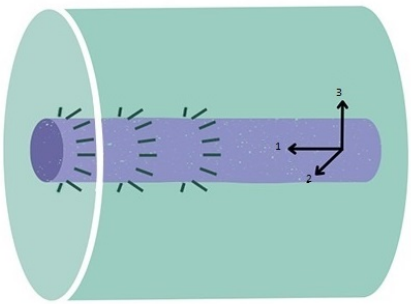


Figure 2: Representation of CNTs grow radially around a carbon fiber

Manufacturing FFC is a challenging process compared to traditional composite materials. [Shan et al., 2013] introduced a new technique to significantly improve carbon-reinforced polymers' out-of-plane properties. A new spraying technique is E20 for coating carbon surfaces with CNT. Also, chemical vapor deposition (CVD) is used to manufacture this material. If the CNT is not grown with these unique techniques, mechanical properties become very poor. It decreases beyond the

properties of conventional carbon fiber composites.
The area has many challenging problems, such as preparation, synthesis, processing, and characterization. The study focuses on the characterization of hybrid composites with the help of the computational homogenization method. A two-step homogenization approach is followed to understand the overall macroscopic behavior of the composite. In the first step, the interphase region consisting of a polymer matrix and radially aligned CNTs is homogenized using the micro-mechanics-based Mori-Tanaka method. After obtaining the homogenized properties of the interphase, 3-phase FFC will be homogenized using the Finite Element Method. ABAQUS [ABAQUS, 2014] and MATLAB programs are used to implement the homogenization method.

METHOD

CNTs and carbon fiber are considered transversely isotropic linear elastic, while epoxy is assumed to be isotropic linear elastic. Material properties are taken from the study of [Tsai et al., 2010] and can be seen in Table 1. CNTs are considered inclusions in the epoxy matrix. Furthermore, between the constituents, perfect bonding is assumed. Therefore, the Mori-Tanaka approach [Qiu et al., 1990] can be used to calculate the effective properties of the heterogeneous material. Effective elasticity tensor is defined by

$$C^{eff} = C^m + \sum_{\alpha=1}^{B} v_\alpha (C^\alpha - C^m) : A^\alpha, \tag{1}$$

where α, B, v_α, C^m, and C^α respectively represent the inclusion number, the total number of inclusions, the volume fraction of the α^{th} inclusion, the fourth-order elasticity tensor of the matrix and inclusion. The strain concentration tensor A^α is defined as

$$A^\alpha = A^\alpha_m : \left[v_m \mathbb{I} + \sum_{\beta}^{M} v_\beta A^\beta_m \right]^{-1}, \tag{2}$$

where v_m and $\mathbb{I}$ represent the volume fraction of the matrix and the fourth-order identity tensor, respectively. A^α_m is defined as

$$A^\alpha_m = \left[\mathbb{I} + S^\alpha : (C^m)^{-1} : (C^\alpha - C^m) \right]^{-1}, \tag{3}$$

In Eqn. 3, S^α is the Eshelby tensor [Qiu et al., 1990]. In this study, the Mori-Tanaka method is implemented for cylindrical CNT. Thus, the Eshelby tensor for cylindrical inclusion in the isotropic matrix should be used in the equations. For a needle or circular cylinder, the Eshelby tensor is defined as,

$$\begin{aligned}
S_{1111} &= 0, \\
S_{2222} = S_{3333} &= \frac{5 - \nu_0}{8(1 - \nu_0)}, \\
S_{2233} = S_{3322} &= \frac{4\nu_0 - 1}{8(1 - \nu_0)}, \\
S_{2211} = S_{3311} &= \frac{\nu_0}{2(1 - \nu_0)}, \\
S_{1122} = S_{1133} &= 0, \\
S_{2323} &= \frac{3 - 4\nu_0}{8(1 - \nu_0)},
\end{aligned}$$

$$S_{1212} = S_{1313} = \frac{1}{4}, \tag{4}$$

where ν_0 is the Poisson's ratio of the isotropic matrix.

Table 1: The engineering material properties of carbon fiber, CNT, and epoxy.

Material	E_I [Pa]	E_T [Pa]	G_I [Pa]	ν_I [-]	ν_T [-]
Carbon Fiber	230×10^9	15×10^9	25×10^9	0.29	0.46
CNT	759×10^9	425×10^9	596×10^9	0.27	0.20
Epoxy	3×10^9	3×10^9	1.15×10^9	0.30	0.30

The Mori-Tanaka method calculates the effective elasticity tensor with the volume fraction of the inclusion. When considering the interphase, the CNT interphase region has a graded structure because the volume fraction of the CNTs decreases as it moves away from the fiber surface. To this end, the volume fraction will be computed as a function of the distance to the fiber surface, as shown in Figure 4, and the Mori-Tanaka method should be modified accordingly. Furthermore, the USDFLD subroutine is implemented in ABAQUS to define the material properties of the element integration points as they vary with integration point coordinates in the global coordinate system. The pre-known total CNT volume fraction calculates the local volume fraction of the CNTs in the composite for a given RVE. The total number of CNTs NO_{CNT} is calculated as,

$$NO_{CNT} = \frac{\nu_{CNT} V_{RVE}}{A_{CNT} * l_{CNT}}, \tag{5}$$

where ν_{CNT} is the CNT volume fraction, V_{RVE} is the volume of the RVE, A_{CNT} is the cross-sectional area of a single CNT, and l_{CNT} is the CNT length. Local CNT volume fraction becomes

$$\nu_{CNT_{local}}(r) = \frac{A_{CNT} NO_{CNT}}{2\pi r l_{RVE}}, \tag{6}$$

where l_{RVE} is the RVE length defined in Figure 3, and r is the distance of the integration point to the carbon fiber center.

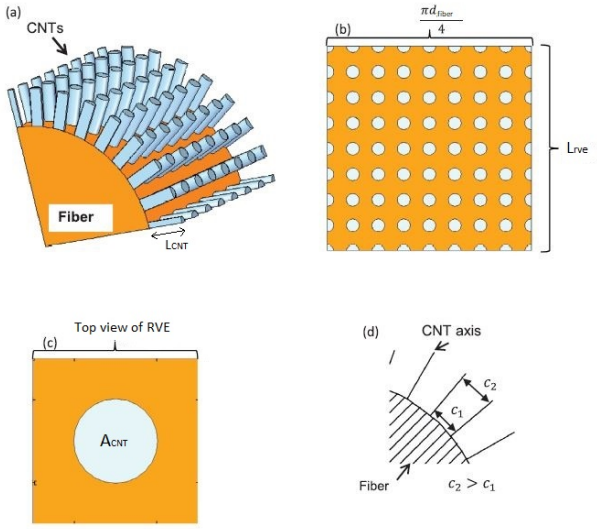


Figure 3: Representation of FFC: (a) 3D RVE of FFC; (b) CNTs on fiber surface from top view; (c) RVE of a single CNT; (d) Reduction in CNT volume fraction representation[Sabuncuoglu et al., 2018]

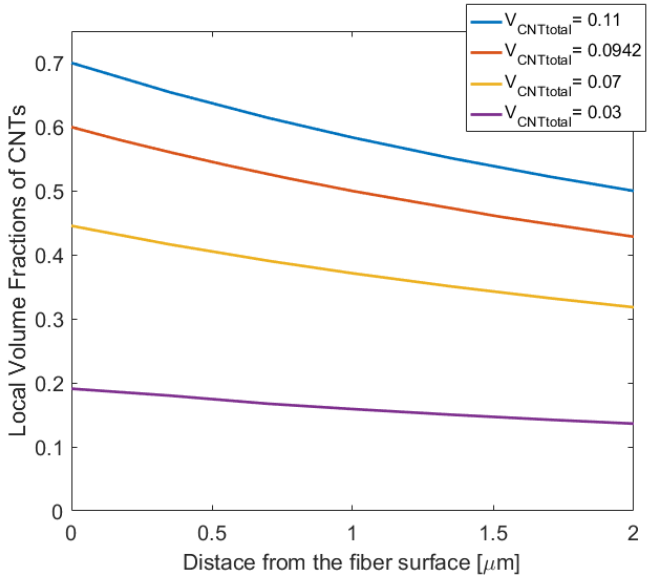


Figure 4: Variation of local volume fraction of CNTs in interphase as a function of distance from the fiber surface.

After the interphase homogenization, results from the Mori-Tanaka method are implemented as material properties in ABAQUS finite element solver for every integration point of finite elements located in the interphase region. Since the FFC has a transversely isotropic structure, four different loadings are applied; normal loading in the axial direction, normal loading in the transverse direction, simple shear loading perpendicular to the fiber direction, and simple shear loading parallel to the fiber direction. In addition, the uniform displacement boundary condition is applied to the representative volume element (RVE) (Figure 5) in computational homogenization, as in Table 2. Linear displacement boundary condition (Dirichlet condition [Nguyen et al., 2012]) defines the displacement field on the boundary of the RVE that assumes the strain is uniform over the boundary of the RVE. The displacement field is defined as on the RVE:

$$\mathbf{u} = \langle \varepsilon(\mathbf{u}) \rangle \mathbf{x} \quad on \quad \Gamma, \tag{7}$$

where $\varepsilon(\mathbf{u})$ is the macroscopic strain filed and $\mathbf{x}$ is the position vector of a point on the boundary Γ. After completing the finite element analysis, each integration point's stresses, strains, and volume are exported as an ABAQUS report file. Finally, a subroutine in MATLAB is written to calculate the homogenized properties of the FFC with the ABAQUS report file.

Table 2: Uniform displacement boundary conditions and responses in FEM analysis.

Loading Direction	Strain	Stress (Response)
Axial Loading (11)	$\{\varepsilon_{11}, 0, 0, 0, 0, 0\}$	$\{\sigma_{11}, \sigma_{22}, \sigma_{33}, 0, 0, 0\}$
Transverse Loading (22)	$\{0, \varepsilon_{22}, 0, 0, 0, 0\}$	$\{\sigma_{11}, \sigma_{22}, \sigma_{33}, 0, 0, 0\}$
Simple Shear Loading (23)	$\{0, 0, 0, \gamma_{23}, 0, 0\}$	$\{0, 0, 0, \tau_{23}\, 0, 0\}$
Simple Shear Loading (12)	$\{0, 0, 0, 0, 0, \gamma_{12}\}$	$\{0, 0, 0, 0, 0, \tau_{12}\}$

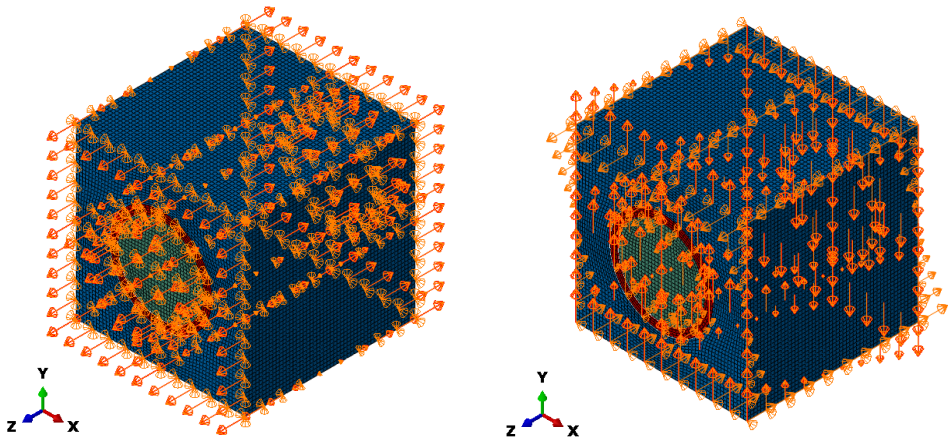


Figure 5: Representative finite element models of normal loading in the axial direction and simple shear loading parallel to the fiber direction.

In order to calculate the elastic coefficients of the materials, the stress-strain relation is used, as shown in Eqn. 5. The fourth-order elasticity tensor has 81 components. Due to the major and minor symmetries of the tensor, the number of independent coefficients reduces to 21 for an anisotropic material. In the study, the FFC is considered a transversely isotropic material. Thus, the number of independent coefficients reduces to 5. Normal loading in the axial direction is applied to the finite element model to compute the C_{11} and C_{12}. Normal loading in the transverse direction is applied to calculate C_{22} and C_{23}. Moreover, shear loadings perpendicular to the fiber direction and parallel to the fiber direction are applied to compute the last unknown elastic coefficient, C_{55}.
In Table 3, $E_I, E_T, G_I, G_T, \nu_I$, and ν_T stand for; the tensile elastic modulus, the transverse elastic modulus, the in-plane shear modulus, the out-of-plane shear modulus, the in-plane Poisson's ratio, and the out-of-plane Poisson's ratio, respectively. The in-plane properties are the properties of the plane parallel to the fiber, and the out-of-plane properties are the properties of the plane perpendicular to the fiber for transversely isotropic materials.

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{12} & C_{23} & C_{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{C_{22}-C_{23}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{55} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix} \tag{8}$$

RESULTS

The engineering properties of the homogenized fuzzy fiber composite (FFC) with a CNT volume fraction of 0.07 and fiber-reinforced polymer (FRP) are presented in Table 3. As seen from the obtained results, grafting CNT on the fiber increases the transverse and shear moduli of the material between 20% and 30%, while the tensile elastic modulus changes less than 1%. The interfacial bonding between fiber and the matrix is very critical for the out-of-plane properties of the composite material. As aforementioned, bristled interphase increases the fibers' surface area, providing more effective load transfer between the fiber and matrix. The results show that the composite system's transverse properties are enhanced by adding CNTs.

Table 3: Comparison of homogenized elastic constants of FRP and FFC.

	E_I [Pa]	E_T [Pa]	G_I [Pa]	G_T [Pa]
FFC	47.9×10^9	5.1×10^9	2.2×10^9	1.8×10^9
FRP	47.5×10^9	4.2×10^9	1.7×10^9	1.5×10^9
Difference (%)	0.8	22.2	27.1	24.1

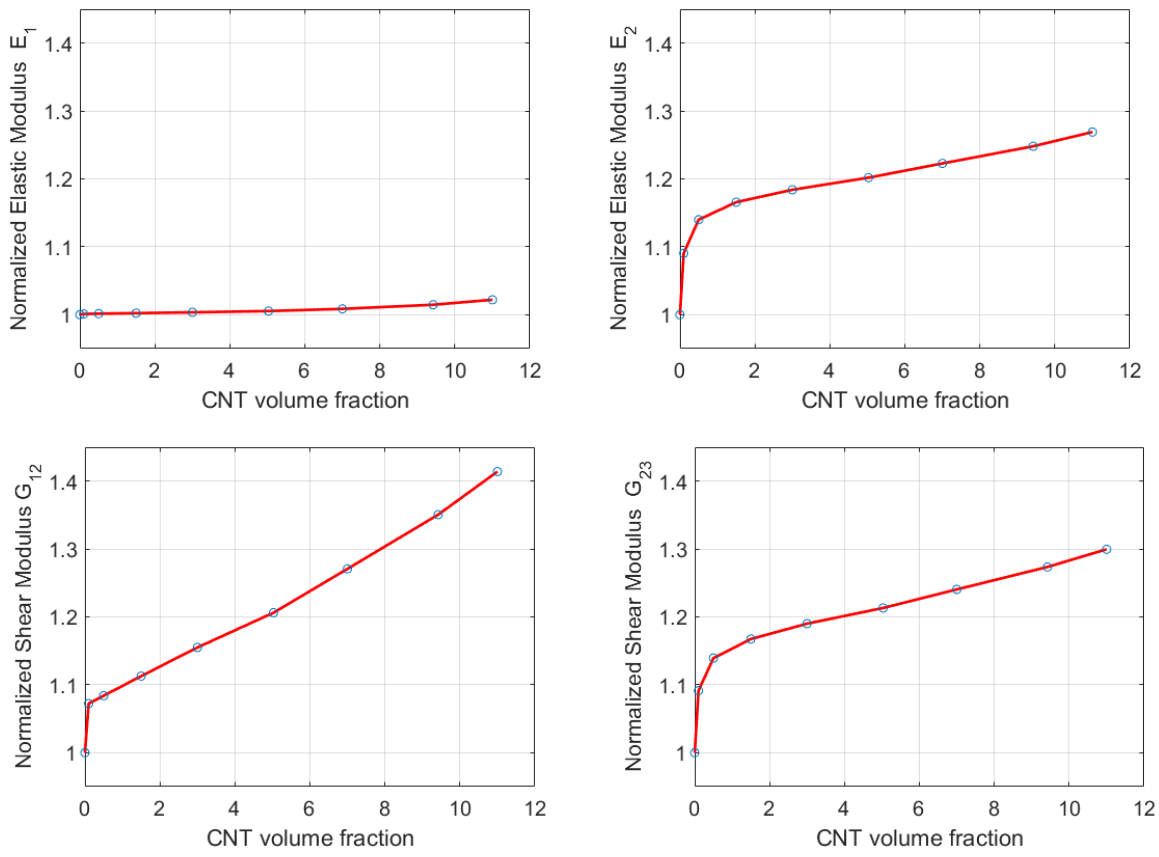


Figure 6: Effects of CNT volume fraction in interphase on normalized engineering constants.

A study of the effects of CNT volume fraction is performed for a fixed volume fraction of fiber. The CNT length and the cross-sectional area of CNTs are also fixed. Only the number of the CNT is increased to increase the volume fraction. As the CNT volume changes, the matrix volume fraction changes, respectively. The effects of the CNT volume fraction on engineering constants are presented in Figure 6. The horizontal axes in Figure 6 are the local volume fraction of CNT in the interphase.

The elastic and shear modules are normalized through the carbon fiber reinforced composite without no CNT growth on the fiber. E_1, E_2, G_{12}, and G_{23} are the tensile elastic modulus, transverse elastic modulus, shear modulus parallel to the fiber direction, and shear modulus perpendicular to the fiber direction, respectively. It can be concluded from the results that increasing the volume fraction of CNT stiffens the interphase, which reveals that effective engineering constants of the FFC increase with the CNT volume fraction.

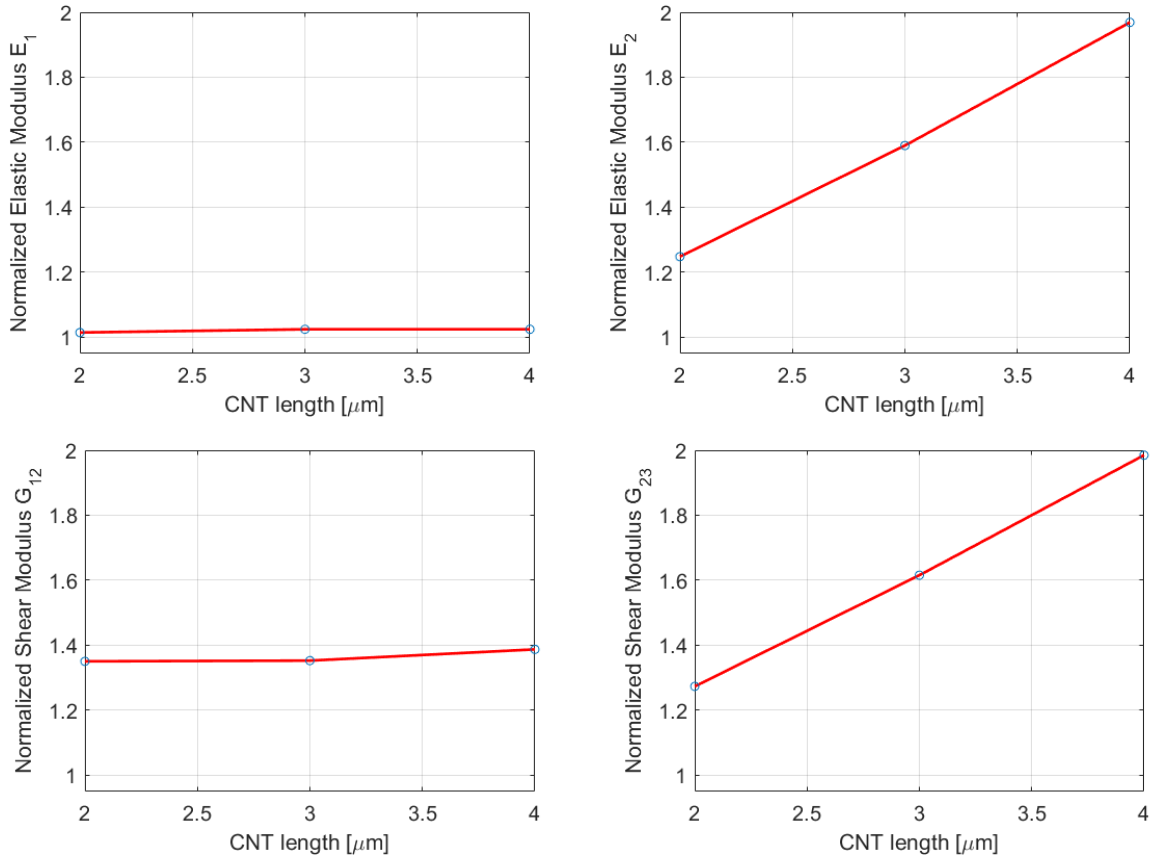


Figure 7: Effects of CNT length on engineering constants.

CNT length's effects on engineering constants are studied for a fixed volume fraction of fiber, CNT, and matrix. Only the length of the CNTs is changed. The effects of CNT length on engineering constants are presented in Figure 7. Increasing the length of CNT while keeping the total volume fraction the same thickens and softens the interphase at the same time. It can be concluded from the results that increasing the CNT length increases the transverse elastic moduli and shear moduli by about 60%, while the tensile elastic moduli and shear moduli change by less than 2%.

CONCLUSION

In this study, the effective elastic properties of the FFC were studied using a two-step computational homogenization approach. The first step uses a micromechanics-based Mori-Tanaka method to homogenize functionally graded interphase. Using the Mori-Tanaka method gives very accurate results and is advantageous regarding computational cost. In the second step, an RVE is constructed for 3-phase fuzzy fiber and homogenized using FEM. The effective properties are compared with grafting CNTs on fiber with a base fiber-reinforced polymer composite. The effects of CNT volume fraction and length were studied. The following conclusions can be drawn:

- Homogenizing the hybrid composites with the computational homogenization approach can be costly due to the functionally graded interphase. However, the proposed two-step homogenization approach provides a cost-effective solution.
- Grafting CNTs on the fiber surface increases the effective properties of the composite material, which increases the fiber's surface area, providing more effective load transfer between the fiber and the matrix.
- Parametric studies reveal that increasing the volume fraction of CNTs and the length of the CNTs enhance the effective elastic properties of FFC.

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