

Prediction of Elastic Constants of the Fuzzy Fibre Reinforced Polymer Using Computational Micromechanics

Marzena Pawlik, Yiling Lu

Department of Mechanical Engineering and the Built Environment, University of Derby,
Derby, United Kingdom

e-mail: m.pawlik@derby.ac.uk, y.lu@derby.ac.uk

Abstract. Computational micromechanics is a useful tool to predict properties of carbon fibre reinforced polymers. In this paper, a representative volume element (RVE) is used to investigate a fuzzy fibre reinforced polymer. The fuzzy fibre results from the introduction of nanofillers in the fibre surface. The composite being studied contains three phases, namely: the T650 carbon fibre, the carbon nanotubes (CNTs) reinforced interphase and the epoxy resin EPIKOTE 862. CNTs are radially grown on the surface of the carbon fibre, and thus resultant interphase composed of nanotubes and matrix is transversely isotropic. Transversely isotropic properties of the interphase are numerically implemented in the ANSYS FEM software using element orientation command. Obtained numerical predictions are compared with the available analytical models. It is found that the CNTs interphase significantly increased the transverse mechanical properties of the fuzzy fibre reinforced polymer. This extent of enhancement changes monotonically with the carbon fibre volume fraction. This RVE model enables to investigate different orientation of CNTs in the fuzzy fibre model.

1. Introduction

Fibre reinforced polymers (FRP) enjoy increasing applications, and mechanical properties are key to exploit their full potential. Traditionally, mechanical properties of composites are extracted from experimental testing; however, this process is very tedious and expensive. Computational micromechanics becomes an efficient tool to predict elastic constants of FRP. This numerical approach can tailor the composition and structure of composites to meet specific requirements even before a physical sample is prepared.

Computational micromechanics analyses the composite properties at the constituent level using a representative volume element (RVE) [1]. The RVE is theoretically the smallest volume representing the whole material. Most composites have fibres randomly arranged in the microstructure; however, a good approximation of elastic constants can be achieved by periodic microstructures [2]. Generally, three types of RVE models with cylindrical [3], square [4] and hexagonal [5] fibres arrays appear in the literature. These models have been successfully applied to the determination of the FRP properties, where the proposed RVE models consist of two phases such as the fibre and matrix. Recently, the effects of an interphase have attracted a lot of interest. The interphase is defined as a thin layer between fibre and matrix which is usually created by the protective coating of the fibre and manufacturing processes [6].



Kari et al. [7] observed that overall material properties of the unidirectional lamina were significantly affected by interphase, particularly in the transverse direction. Xu et al. [8] discussed the results of volume fraction and stiffness of the interphase on the engineering elastic constants of the composite. In most works, the interphase is simplistically treated as isotropic [7-11].

Carbon nanotubes (CNTs) discovered by Iijima [12] have long been tried as the enhancer of nanocomposites because of superior and multi-functional properties and the axial Young's modulus exceeding 1 TPa [13]. In recent years, CNTs have also been applied in FRP by growing [14-17] or spraying onto the fibre surface [18]. Coated with CNTs carbon fibres are then embedded in the matrix forming the fuzzy fibre reinforced polymer (FFRP). Experimental studies found that the presence of CNTs increased not only the interfacial shear strength [19] but also material moduli of FFRP. For example, Mathur et al. [20] observed 28% increase in flexural modulus of the FFRP over the pure carbon fibre based composites.

Promising experimental results have motivated researchers to study the effects of CNTs on the FFRP properties by analytical and numerical approaches [21-28]. For example, Kulkarni et al. [21] estimated mechanical properties of a nano-reinforced laminated composite with two different volume fractions of CNTs using multiscale modelling and cylindrical RVE micromechanical method. Numerically predicted transverse modulus was 40% higher than experimentally determined value. Ray et al. [22] proposed a shear lag model to obtain the response of the CNTs coated piezoelectric fibre reinforced composites. Kundawal and Ray [23] developed a method to evaluate elastic constants of continuous fuzzy fibre composites using mechanics of materials combined with Mori-Tanaka approach. Whereas, Chatzigeorgiou et al. [24] characterised fuzzy fibre reinforced composites considering various CNTs volume fractions and lengths. Ren et al. [25] experimentally and computationally estimated the piezoresistivity of fuzzy fibre reinforced polymer by 3-D FEM multiscale model. More recently, Rafiee and Ghorbanhosseini [26] applied a stochastic multi-scale model to obtain mechanical properties of FFRP with randomly orientated CNTs on the fibre surface.

In the present work, the RVE with hexagonal fibres array is used for numerical simulation to predict the properties of the fibre reinforced polymer with the concept of the CNTs reinforced interphase. The influence of the interphase properties on the response of the FFRP is analysed for a various carbon fibre volume fractions. Two types of models: with and without the CNTs reinforced interphase are compared to highlight its influence on material properties.

2. RVE method

2.1. Fuzzy fibre polymer – RVE model.

Fig.1a shows a schematic representation of a unidirectional carbon fibre reinforced lamina. The mechanical behaviour of this composite can be effectively studied using the hexagonal RVE model as presented in Fig.1 b. The RVE model contains three phases: the carbon fibre, the CNTs reinforced interphase and the epoxy resin. In the fuzzy fibre, CNTs are radially grown on the surface of the carbon fibre (Fig.2a); therefore, the CNTs reinforced interphase is composed of the nanotubes and epoxy. The transversely isotropic features of CNTs are taken into account in the reinforced interphase. Their material properties symbols and subscripts follow the local coordinate system $1'-2'-3'$ presented in Fig 2b. Fuzzy fibres are arranged in the unidirectional lamina and follow Cartesian coordinate system with axes denoted by 1-2-3, where, 1 is the carbon fibre direction.

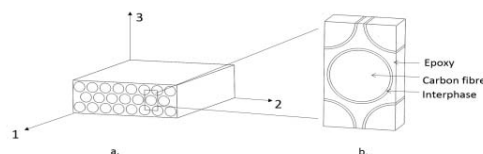
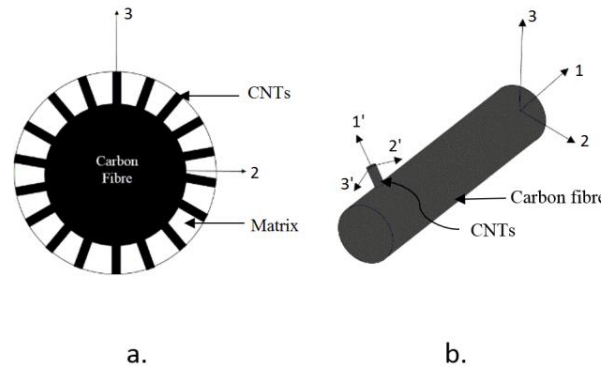


Figure 1. Schematic representations of a. the carbon fibre reinforced polymer, b. the three-phase RVE.**Figure 2.** Schematic illustrations of a. cross-section view of the fuzzy fibre, b. perspective view of the fuzzy fibre.

2.2. Material properties of each phase

Two-phase and three- phase models are investigated to highlight the effects of the CNTs-reinforced interphase on the mechanical properties of the FFRP. In the two-phase model, mechanical properties of the transversely isotropic T650 carbon fibre and the isotropic EPIKOTE 862 epoxy resin are selected (Table I) [24]. Properties of the transversely isotropic carbon fibre are assigned according to the lamina coordinate system. Dimensions of the RVE are calculated based on the fibre volume fraction and fibre diameter (5 μm). For example, for 25 % of carbon fibre volume fraction, height, width and thickness are 8.23, 4.76 and 1.19 μm respectively. Detailed information can be found in [1]. The three-phase model also includes the CNTs reinforced interphase. The “VEORIENT” command is applied to the RVE model to define the orientation of the CNTs. This command allows specifying element orientation to control transversely isotropic material property direction. The CNTs reinforced interphase has a thickness of 2 μm . The average volume fraction of CNTs in the interphase amounts to 42% [24]. As a result of CNTs mechanical characteristics and orientation, the interphase is transversely isotropic. The material properties of the CNTs interphase are taken from literature. Poisson’s ratios are calculated from the bulk moduli provided by [24] (Table II).

Table 1. Material properties of the carbon fibre and epoxy resin.

Matrix : EPIKOTE 862 Resin	
Modulus, E_m	3 GPa
Poisson’s ratio, ν_m	0.3
Fibre: Carbon fibre T650	
Longitudinal modulus, E_{f1}	241 GPa
Transverse modulus, E_{f2}	14.5 GPa
In-plane shear modulus, G_{f12}	22.8 GPa
Transverse shear modulus, G_{f23}	4.8 GPa
In-plane Poisson’s ratio, ν_{f12}	0.27

Matrix : EPIKOTE 862 Resin	
Modulus, E_m	3 GPa
Diameter	5 μm

Table 2. Material properties of the CNTs reinforced interphase.

Interphase : CNTs reinforced interphase	
Longitudinal modulus, $E_{1'}$	298.64 GPa
Transverse modulus, $E_{2'}$	7.01 GPa
In-plane shear modulus, $G_{12'}$	2.81 GPa
Transverse shear modulus, $G_{23'}$	2.52 GPa
In-plane Poisson's ratio, $\nu_{12'}$ ^a	0.1
Out-of-plane Poisson's ratio, $\nu_{23'}$	0.29

a. estimated property

Both models are simulated using ANSYS APDL 17.2. Perfect bonding conditions between each phase are assumed. The meshes generated for the models investigated are 20-node 3-D solid elements (SOLID186). Mesh independent test was accomplished to eliminate the influence of the number of elements on the accuracy of the results. The whole meshed model contains approximately 7000 elements.

Keeping the same properties and dimensions for all constituents, we performed numerical simulations where carbon fibre volume fractions ranging from 0 to 25% for two and three-phase models. Note that 25% carbon fibre volume fraction corresponds to 81% volume fraction of the FFRP model (carbon fibre together with the CNTs interphase).

2.3. Evaluation of elastic constants

The prediction of elastic constants of the fibre-reinforced composite is based on Hooke's law for transversely isotropic materials (1), where C_{ijkl} is a stiffness matrix, and $\bar{\sigma}_{ij}$ and $\bar{\epsilon}_{ij}$ are the volume average stresses and strains respectively. The volume average strains and stresses are obtained by (2), where V is the volume of the RVE.

$$\begin{Bmatrix} \bar{\sigma}_1 \\ \bar{\sigma}_2 \\ \bar{\sigma}_3 \\ \bar{\tau}_4 \\ \bar{\tau}_5 \\ \bar{\tau}_6 \end{Bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{12} & C_{23} & C_{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}(C_{22} - C_{23}) & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{66} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix} \begin{Bmatrix} \bar{\epsilon}_1 \\ \bar{\epsilon}_2 \\ \bar{\epsilon}_3 \\ \bar{\gamma}_4 \\ \bar{\gamma}_5 \\ \bar{\gamma}_6 \end{Bmatrix} \quad (1)$$

The periodic boundary conditions are applied to the RVE model to compute stresses, strains and calculate the overall elastic matrix, C_{ijkl} . The comprehensive description of the periodic boundary conditions can be found elsewhere [1, 2, and 29].

$$\bar{\epsilon}_{ij} = \frac{1}{V} \int_V \epsilon_{ij} dV$$

$$\bar{\sigma}_{ij} = \frac{1}{V} \int_V \sigma_{ij} dV \quad (2)$$

When the components of the tensor C are known, the five elastic properties of the homogenised material can be calculated (3); where E_1 and E_2 represent the longitudinal and transverse moduli, ν_{12} and ν_{23} are the in-plane and out-of-plane Poisson's ratios, G_{12} is the in-plane shear modulus, and G_{23} is out-of-plane shear modulus. Calculated mechanical properties for both models are compared and presented in Fig. 3 to 6.

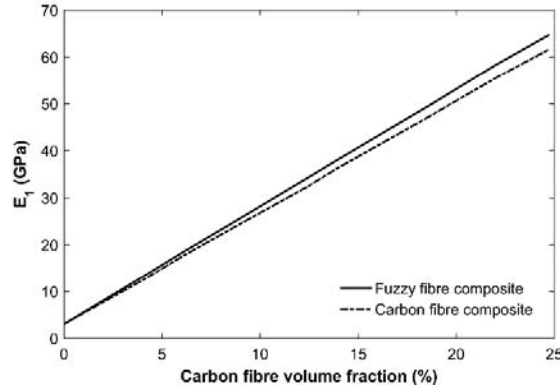


Figure 3. Longitudinal modulus versus carbon fibre volume fraction.

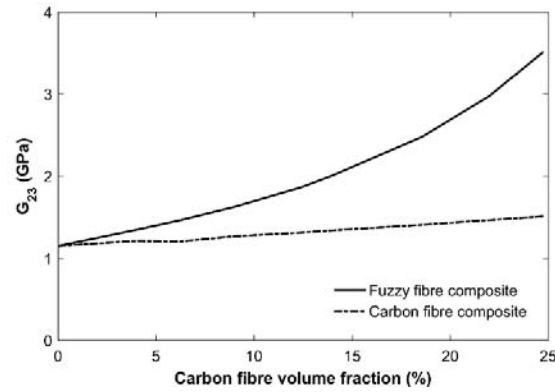


Figure 4. Transverse modulus versus carbon fibre volume fraction.

$$\begin{aligned}
 E_1 &= C_{11} - 2C_{12}^2/(C_{22} + C_{23}) \\
 E_2 &= [C_{11}(C_{22} + C_{23}) - 2C_{12}^2](C_{22} - C_{23})/(C_{11}C_{22} - C_{12}^2) \\
 \nu_{12} &= C_{12}/(C_{22} + C_{23}) \\
 \nu_{23} &= [C_{11}C_{23} - C_{12}^2]/(C_{11}C_{22} - C_{12}^2) \\
 G_{12} &= C_{66}
 \end{aligned} \tag{3}$$

3. Results

3.1. Longitudinal modulus

Fig.3 presents longitudinal modulus, E_1 , versus carbon fibre volume fraction of fuzzy fibre and carbon fibre composites. In both cases, for 0% carbon volume fraction results started from 3 GPa, which was the modulus of the pure matrix. For 25% of carbon volume fraction in the fuzzy fibre material, the

longitudinal modulus increased up to 65 GPa. For the same volume fraction of composite without the interphase, the modulus was 61.7 GPa. The nearly linear relationship between modulus and volume fraction was obtained for both models. Results for two and three-phase models were close to each other.

3.2. Transverse modulus

Transverse modulus, E_2 , for the two-phase model was almost insensitive to the increment of carbon fibre volume fraction (Fig.4). However, the significant increase was observed for the FFRP. Transverse modulus increased from 3 GPa, for 0% volume fraction, up to 10.4 GPa for 25% of carbon fibre volume fraction. In comparison to the two-phase composite, the presence of CNTs interphase increased transverse modulus more than 200%, when volume fraction reached above 20%. The improved performance of FFRP is attributed to the high axial stiffness of the CNTs which are orientated in the transverse direction of the fibre.

3.3. Shear moduli

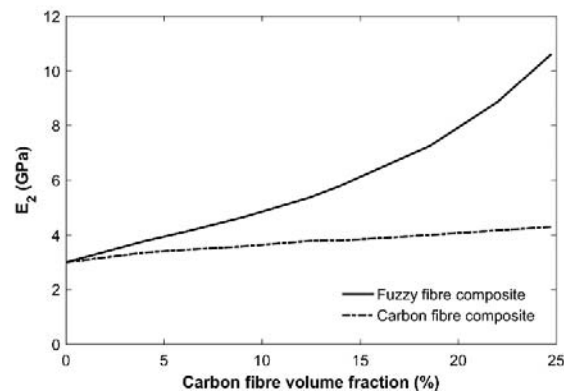


Figure 5. Out-of-plane shear modulus versus carbon fibre volume fraction.

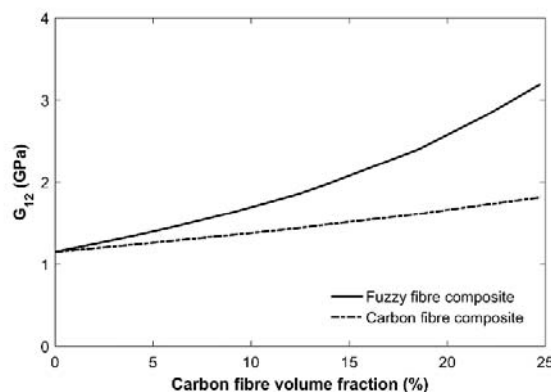


Figure 6. In-plane shear modulus versus carbon fibre volume fraction.

Both similar curves for in-plane and out-of-plane shear moduli were observed in Fig.5 and 6. Shear moduli, G_{12} and G_{23} , values for carbon fibre model were nearly insensitive to the change of the carbon fibre volume fraction. Significant increases were observed in the case of the fuzzy fibre. Up to 10 % of carbon fibre volume fraction, the increase was almost linear. Above 10%, shear moduli grow exponentially. For 25 % of carbon fibre volume fraction, shear moduli enhanced more than twice.

4. Discussion

Numerical results predicted by the hexagonal RVE perfectly match analytical results calculated by composite cylinders method [24], which are not shown on the graphs. Kundawal et al. [23, 27] established similar trends in carbon fibre volume fraction, and effective elastic coefficients of fuzzy fibre reinforced composites predicted by mechanics of materials combined with Mori-Tanaka approach.

The purpose of coating fibres with nanofillers is to strengthen the interphase between the fibre and matrix. Numerical results show a significant improvement of properties in the transverse direction. Transverse properties of the carbon fibre-reinforced composites are governed by matrix-dominant properties and are considerably lower in comparison to longitudinal. The presence of CNTs in the matrix surrounding the carbon fibre enhances the performance of the FFRP. This enhancement is attributed to the unique orientation where axial direction of the CNT is aligned with the transverse direction of the carbon fibre. An experimental study [13] supports these findings. According to Kulkarni et al. [21], the transverse elastic modulus can usually be improved about three times with respect to the value of the pure matrix. In this study, for 25 % carbon fibre volume fraction, the transverse modulus increased more than twice. The achieved increase depends on the volume fraction of the CNTs in the interphase and also on the quality of manufacturing process.

Contrarily, the presence of the CNTs radially grown on the surface of carbon fibre has negligible influence on the longitudinal modulus of the fuzzy fibre composite. The highest improvement of longitudinal modulus is observed for the 25% carbon fibre volume fraction and results in only 5% increase. This lower increase is associated with weaker properties of the interphase in the carbon fibre direction (1-direction in global coordinate system) which is caused by lower transverse properties of the single nanotube.

In the case of fuzzy fibre, cylindrical RVE is more commonly used due to the axisymmetric nature [21]. However, the hexagonal RVE model frees us from the cylindrical coordinate system which is required by the analytical way. This model enables to study a various distribution and directions of nanofillers, for example, the graphene sheets parallel aligned to the fibre surface or randomly distributed in the reinforced interphase [28].

The main limitation of this study is the assumption of perfectly straight CNTs, evenly distributed on the fibre surface. In reality, during the manufacturing process, some defects may occur. Moreover, the thickness of CNTs interphase may not be uniform throughout the fibre. These problems will be considered in the future work.

5. Conclusion

To sum up, our work has investigated the effects of the CNTs interphase on the fuzzy fibre composite using computational micromechanics. The RVE with hexagonal fibre array successfully predicted elastic constants of the fuzzy fibre composite. The results indicate that CNTs have a significant influence on transverse properties of the FFRP. This study provides the framework to study the fibre-reinforced composite with the existence of the nano-reinforced interphase. This numerical model allows dealing with arbitrary shapes of fibres which cannot always be tackled analytically. The developed code can simply and promptly calculate the required properties. Direction-dependent properties of the interphase and fibres can be readily implemented.

6. Acknowledgment

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