Effect of geometrical configurations of fiber on the effective properties of unidirectional carbon-fiber/epoxy composite

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Abstract. Knowing the effective of both mechanical and thermal properties of composite materials allows researchers to improve their behavior and increasing its reliability. In this study, a simplified micromechanical approach is used to modelling and analysis the unidirectional carbon-fiber/epoxy composite performances. The principle objective of this work is to evaluate the effect of the fiber geometrical configurations on the effective mechanical properties and the thermal expansion's coefficients considering three different geometrical configuration of the fiber. Hence, the unidirectional composite with ellipsoidal fiber is stiffer than others with cylindrical or parallelepipedal fibers. Moreover, the considered configuration wherein the fiber has an ellipsoidal shape leads to lower effective coefficients of thermal expansion corresponding to more cohesion between particles.

Introduction

Fiber composite materials have received tremendous attention in both scientific and industrial communities due to their higher specific strengths and moduli among engineering materials. That's why the research on composites has attracted much attention. Therefore, the mechanical and thermal behavior of composites has been the subject of various studies using different approaches, including experimental investigation, numerical simulations and theoretical modeling.

The effective properties of the fiber composite materials in terms of the properties of the constituents (matrix and reinforcements) can be predicted using the homogenization techniques. Since homogenization models are based on more or less accurate modeling of the microstructure, these models are also called micromechanics models, and the techniques used to obtain approximate values of the composite's properties are called micromechanics methods or techniques.

The accuracy of the micromechanics models and the characteristics affect the effective properties of composites have been the subject of numerous publications.

The micromechanical models suggested in the literature to predict the effective elastic characteristics have been discussed in the review of Vignoli et al [1, 2]. In [3], Raju et al, have analyzed the limitations of these models in their review of micromechanical models used for predicting the effective mechanical properties of reinforced polymer matrix composite. As well as, the authors in [4, 5] have presented a review of some notable micromechanics-based models showing their limitations and presenting a novel and efficient micromechanical computational approach for effective estimation of elastic properties of polymer matrix composites at lower fiber volume fraction. Different micromechanical approaches including analytical and semi-analytical models and 2D and 3D FE approaches methods for the prediction of the stiffness and strength of a unidirectional lamina have been focused and the obtained results have been compared with experimental results available in the literature [6]. Moreover, based on a representative volume element method, micromechanical and thermal properties have been examined by Patnaik et al. [7] for glass-fiber reinforced polymer composites for which the experimental results agreed well with the finite element model. In [8], the authors have proposed a novel approach to calculate the effective thermal conductivities of fiber reinforced composite materials. They proved their approach by comparing the obtained results with the experimental data presented in the literature.

The effect of different parameters on the effective mechanical properties and thermal expansions has been the subject of several researches. Thereby, it has been demonstrated that the effective properties dependent on a number of parameters, including fiber orientation, volume fractions of fibers, array of fibers, and material properties of their constituents. The authors have examined, using a simplified micromechanical model, the effect of volume fraction and constituent properties on the effective longitudinal, transverse, and shear properties of several types of unidirectional composites [9]. Likewise, Makarian and Santhanam in [10] have used the micromechanical model to show the effect of porosity on the elastic and shear modulus, thermal conductivity, and the thermal expansion while accounting for the comparison between the accuracy of the 3D simulations and the 2D FE simulations. Further, the authors in [11] have studied the effects of the reinforcement shape, size, spatial orientation and interphase strength on the mechanical behavior showing the analytical and computational micromechanical methods to evaluate the mechanical properties of particulate reinforced metal matrix composites. The influence of the thickness and the modulus of the interphase as well as the effect of the interphase Poisson's ratio on the effective elastic properties of the composite have been the results of numerical and experimental study in [12]. Besides, the effect of micromechanics models on mechanical property predictions for short fiber composites is discussed in [13]. In addition, the effective elastic properties of fiber reinforced composites materials have been studied with high fiber volume fraction where the fibers are distributed randomly over the transverse cross-section wherein the authors have found that the RVE elastic moduli with randomly distributed fibers are greater than those with periodically distributed fibers.

Motivated by these works, the aim of the present study is to investigate numerically the effect of geometrical configuration of fiber on the effective mechanical properties and thermal expansions.

Methodology

Theoretical formulation. The composites materials considered for this study is a unidirectional fiber for which this latter is considered of different geometrical configurations. However, the fiber is of infinite length, embedded in an isotropic matrix

The unidirectional fiber reinforced composite may be considered to be orthotropic. One plane of symmetry is perpendicular to the fiber direction, and the other two are parallel to the fiber direction and orthogonal among themselves. In this case, 3D Hooke's law is given by [14]:

$$\begin{Bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \sigma_4\\ \sigma_5\\ \sigma_6\end{Bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0\\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0\\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0\\ 0 & 0 & 0 & C_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & C_{55} & 0\\ 0 & 0 & 0 & 0 & 0 & C_{66}\end{bmatrix} \begin{Bmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \gamma_4\\ \gamma_5\\ \gamma_6\end{Bmatrix} \tag{1}$$

Where σij and τ_{ij} are normal and shear components of stress, respectively, ε_i and γ_i are the normal and shear components of strain, respectively, and C_{ij} are the components of the stiffness matrix.

The RVE must be subjected to a set of periodic boundary conditions in order to determine the stiffness matrix C of the homogeneous material at the upper scale. This is possible by imposing suitable constraint equations on each pair of homologous nodes belonging to the RVE's opposite faces.

Once the components of the orthotropic tensor C are determined, the elastic properties of the homogenized material including the longitudinal and transversal Young's moduli E_1 and E_2 and the longitudinal shear modulus G_{12} can be computed as follows:

$$E_{11} = C_{11} - 2C_{12}^2/(C_{22} + C_{33}) \quad (2)$$

$$E_{22} = [C_{11}(C_{22} + C_{23}) - 2C_{12}^2](C_{22} - C_{23})/(C_{11}C_{22} - C_{12}^2) \quad (3)$$

$$G_{12} = C_{66} \quad (4)$$

Analogously to the mechanical homogenization, also effective coefficients of thermal expansion can be evaluated through finite element analysis by applying to the opposite faces of the RVE a uniform temperature field $\Delta T = 1^{\circ}C^{\circ}$ that generate a total strain field equal to zero. Therefore, using the Duhamel-Neumann thermo-elastic law, the equivalent CTEs of the resulting homogeneous medium can be expressed as follows (Voigt's Notation): [15, 16]

$$\alpha_{ij} = -\frac{1}{\Delta T} B_{ij}\bar{\sigma}_j \quad \text{with } i,j = 1,2,3 \quad (5)$$

Where B_{ij} are the components of the effective compliance matrix. In order to improve the estimation of effective properties of composites, several analytical and semi-empirical formulas have been derived to evaluate the effective properties. Among analytical theories, the rule of mixture is the most used one in which the effective properties are given by: [1]

$$E_1 = V_f E_{1f} + V_m E_m \quad (6)$$

$$E_2 = E_3 = E_{2f} E_m / V_f E_m + V_m E_{2f} \quad (7)$$

$$G_{12} = G_{12f} G_m / V_f G_m + V_m G_{12f} \quad (8)$$

Where V is the volume, E_1 is the longitudinal Young modulus, E_2 is the transverse Young modulus and G is the shear modulus. The index m corresponds to the matrix property while the index f represents the fiber property.

The coefficients of thermal expansion a_i for a composite in the longitudinal and transverse directions are calculated from the rule of mixture using:

$$\alpha_1 = \frac{V_f \alpha_{1f} E_{1f} + V_m \alpha_m E_m}{V_f E_{1f} + V_m E_m} \quad (9)$$

$$\alpha_2 = \alpha_3 = (1 + \vartheta_m) V_m \alpha_m + \left(1 + \vartheta_{12f} \frac{\alpha_{1f}}{\alpha_{2f}}\right) V_f \alpha_{2f} - \vartheta_{12} \alpha_{11} \quad (10)$$

Where ϑ is the Poisson's ratio. The index m corresponds to the matrix property while the index f represents the fiber property.

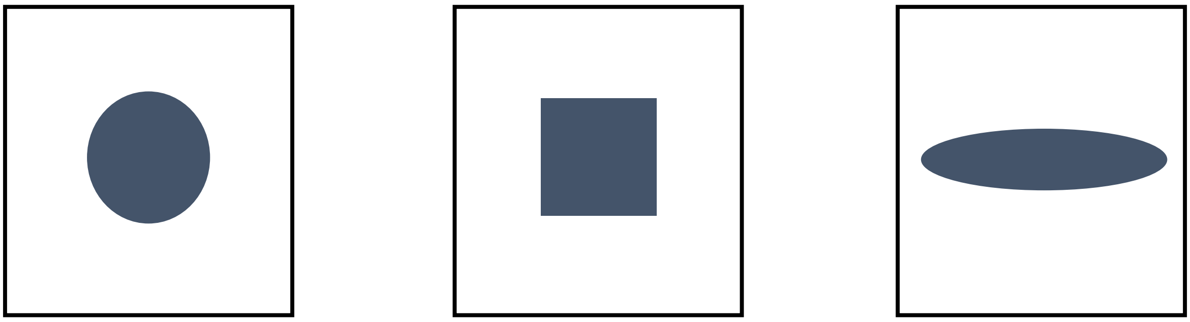
Numerical simulation. In this section, micromechanical modeling using finite element analysis of the effective mechanical properties and thermal expansions of carbon fiber reinforced composite to the main carbon fiber has been carried out. In particular, the influence of the geometrical configuration of the fiber on the mechanical and thermal behavior is investigated. The layers of the laminate are made of T300 carbon fiber and 914C epoxy. The carbon fiber is assumed to be transversely isotropic (modeled as orthotropic), and the epoxy resin is assumed to be isotropic. The material properties of the constitutive phases of the fiber composite in subject of study are listed in Table 1 wherein the index *m* corresponds to the matrix property while *f* represents the fiber property.

***Table1: Material properties of carbon fiber and epoxy resin* [17]**

Material properties	Carbon fiber	Epoxy matrix
Density [Kg/m^3]	1800	110
Young's modulus [*GPa*]	{230, 15, 15}	4
Shear modulus [*GPa*]	{15, 7, 15}	1.48
Poisson's ratios	{0.2, 0.07, 0.2}	0.35
Coefficients of thermal expansion [*1/K*]	{$-6x10^{-7}$, $8.5x10^{-6}$}	$5.5x10^{-5}$

Using finite element software package Comsol Multiphysics, representative unit cell models were constructed for different geometrical configuration of fiber for which the variation of effective properties were studies fro different fiber volume fraction.

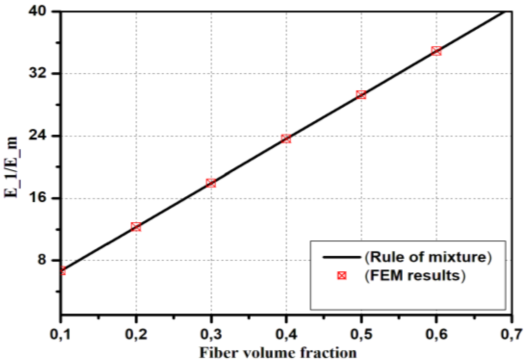
Thus, three cases of study are considered in which the composite material has cylindrical, parallelepipedal and ellipsoidal fibers of infinite length, embedded in a square elastic matrix. For the three cases, the cross-sections of the composite obtained by intersecting the matrix with the orthogonal plane of the fiber axis are circular, square and ellipse, respectively, which clearly shows a periodic microstructure as shown in the "figure 1". Therefore, the characteristic dimension (radius of circle, length of side and the two radius of ellipse) of fiber in each case is defined as a function of the fiber volume fraction and the width of unit cell as mentioned at the "figure 1".



a ***b*** ***c***

Figure 1. Representative volume element of cases of study where the characteristic dimension of fiber of each case is: a: $D_f = 2\sqrt{V_f/\pi l}$; *b:* $l_f = \sqrt{V_f/l}$; *c:* $a_f = 3l/6.5$ *and* $b_f = \sqrt{7V_f/3\pi l^2}$

In order to validate the numerical simulations, the finite element results obtained for the first configuration which constructed as a square RVE with circular fiber geometry will be compared with those obtained using the analytical formulations "Rule of mixture" that presented in the previous section.



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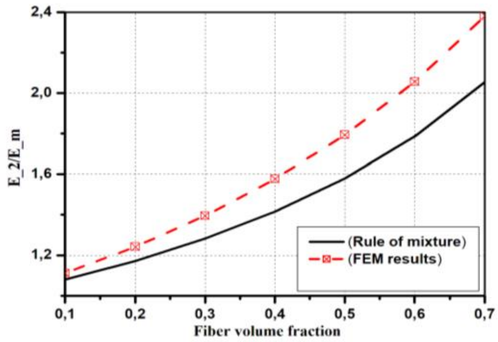

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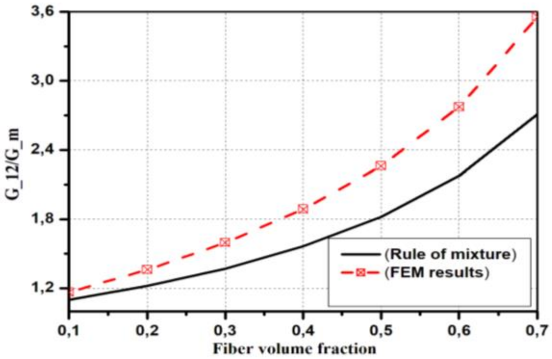
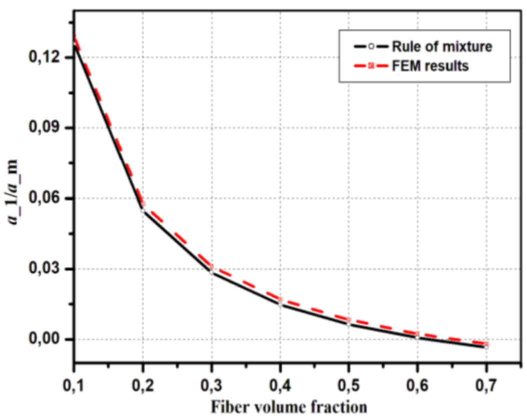


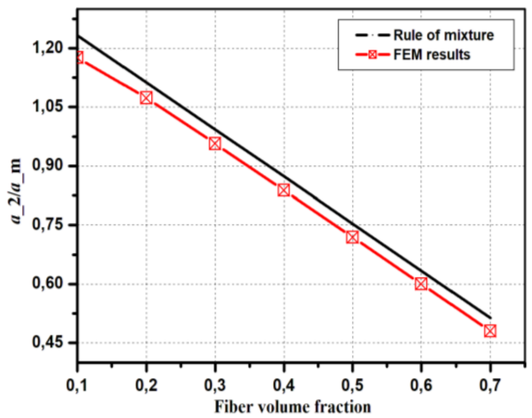
(c)

Figure 2. Validation of the computed elastic properties with different fiber volume fraction -a/ Longitudinal Young's modulus -b/ Transverse Young's modulus -c/ Shear modulus

The comparisons of the elastic properties and the thermal expansions that were determined using finite element software with the results obtained using the Rule of Mixture formulations, are presented in "figure 2" and "figure 3", respectively. It can be seen the good agreement between finite element results and analytical solutions for the computed effective elastic properties as the effective coefficients of thermal expansions.



(a)



(b)

Figure 3. Validation of the computed coefficients of thermal expansion with different fiber volume fraction -a/ Longitudinal Coefficients of thermal expansion -b/ Transverse Coefficients of thermal expansion

Results and discussions

1. Effect of volume fraction on elastic properties.

The longitudinal Young's modulus is the composite's response to a load applied in the direction of the fibers. "figure 4" shows the effect of fiber volume fraction on the effective longitudinal modulus of composite evaluated using finite element analysis with RVEs consists of cylindrical, parallelepipedal and ellipsoidal fibers geometry compared with each other.

It can be observed the increase in linear manner of the longitudinal modulus with increase of fiber content for the three cases of study. As expected, since the fiber is stiffer than the matrix, the greater the fiber volume fraction the higher the stiffness of the composite.

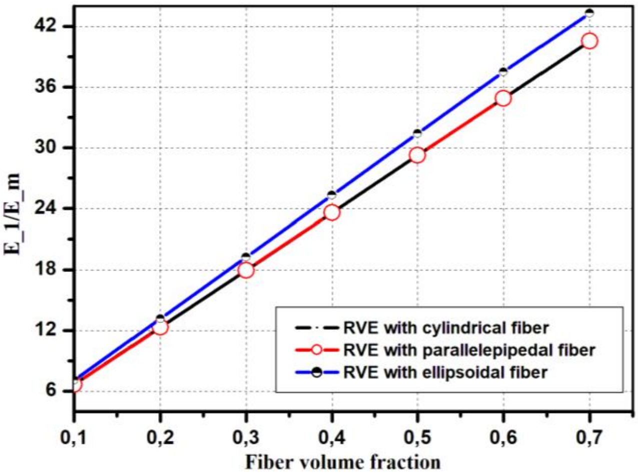


Figure 4. Longitudinal Young's modulus with respect to fiber volume fraction for different geometrical configurations of fiber.

As can be seen, the results obtained for the RVE with cylindrical fiber are equals to those achieved using parallelepipedal fibers. In contrast, there is a significant difference between the results obtained for the third configuration and the other two configurations, where the values obtained for an ellipsoid fiber are greater than those obtained for parallelepipedal and cylindrical fibers which can be reach a rate of about 7 % of difference.

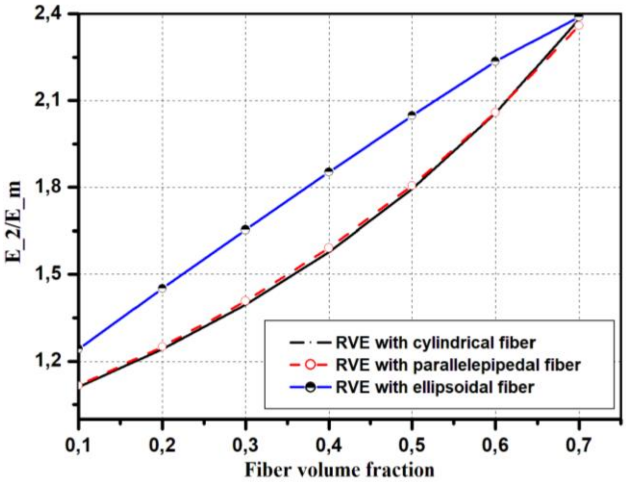


Figure 5. Transverse Young's modulus with respect to fiber volume fraction for different geometrical configurations of fiber.

The evolution of the effective transverse Young's modulus with respect to the fiber volume fraction, for the three different configurations defined above, is shown in the "figure 5". As expected, the transverse Young's modulus increases with increase in fiber volume fraction. However, it's clear from the "figure 5" that the effective modulus obtained in the configuration 1 is closely to that obtained with configuration 2 while it takes higher values, relatively, in the third configuration. The effective transverse Young's modulus evaluated for a RVE with ellipsoid fiber is higher than it in the other cases wherein the VER with cylindrical or parallelepipedal fibers. This difference may take a maximal rate of 15%.

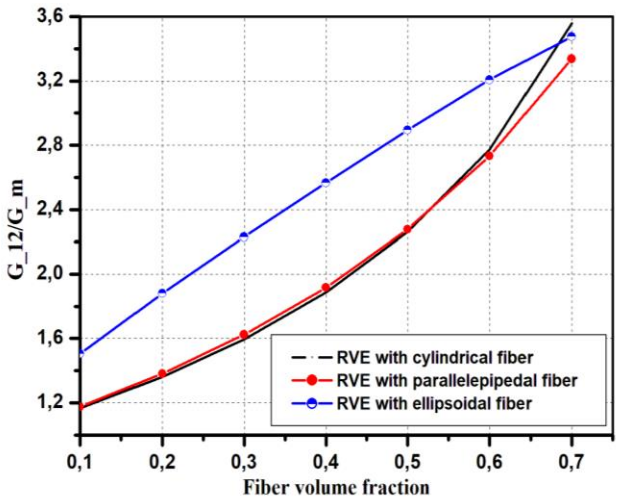


Figure 6. In-plane shear modulus with respect to fiber volume fraction for different geometrical configurations of fiber.

The "figure 6" shows the variation of the effective in-plane shear modulus according to the fiber volume fraction for the three geometrical configurations. As indicated in the figure, the shear modulus increases considerably with the fiber content. This is not surprising, given that the transverse stresses are much more inhomogeneous than those along the fiber. Presumably, the maximum values of the effective shear modulus, relatively, are found for the third configuration. However, a concordance between the results of a RVE with cylindrical fiber and a RVE with parallelepipedal fiber proved by a minimum rate of difference contrary to the results obtained for the configuration where the RVE have an ellipsoidal fiber.

2. Effect of volume fraction on thermal expansions:

The property of a material to transfer heat in parallel to the direction of the fibers is known as longitudinal coefficient of thermal expansion of composite.

The "figure 7" depicts the influence of fiber content on the measure of the effective longitudinal coefficient of thermal expansion using finite element analysis for the three configurations defined previously.

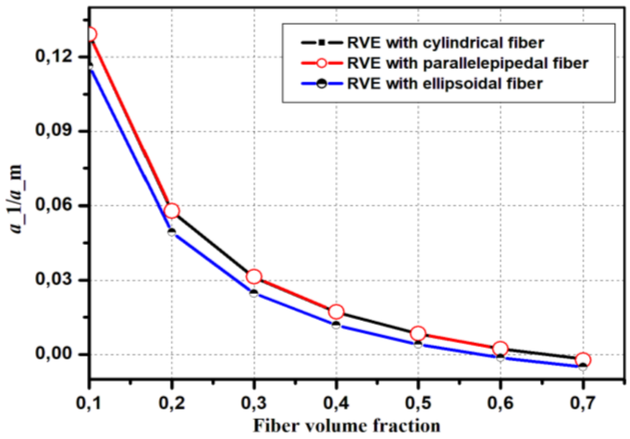


Figure 7. Longitudinal coefficient of thermal expansion with respect to fiber volume fraction for different geometrical configurations of fiber.

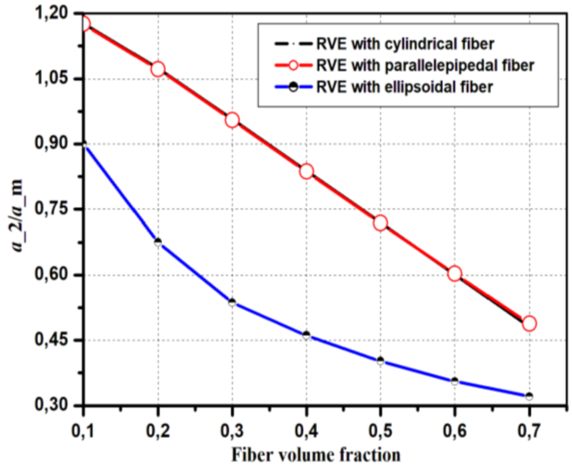


Figure 8. Transverse coefficient of thermal expansion with respect to fiber volume fraction for different geometrical configurations of fiber.

As it clearly appears from the "figure 7", the effective longitudinal coefficient of thermal expansion decreases with the increase in volume fraction since the fiber thermal conductivity dominates the matrix thermal conductivity. However, the effective measure takes the same values for the two configurations wherein the composite with fiber of cylindrical fiber and with parallelepipedal fiber although it takes lower values, relatively, for the third configuration in which the fiber has an ellipsoidal shape. Transverse coefficient of thermal expansion of a composite is the ability of a material to conduct heat perpendicular to the fibers. The effect of fiber volume fraction on the effective transverse coefficient of thermal expansion is shown in "figure 8" using finite element analysis with the three RVEs of different fiber geometry.

As can be seen from the "figure 8", the measure of transverse coefficient of thermal expansion decreases with increase of the fiber content for the three considered configurations. The obtained results for the composite with cylindrical fiber are the same with those obtained in the case of parallelepipedal fiber. In contrast, a significant difference between the effective transverse coefficient of thermal expansion for the third configuration in which the composite have made with ellipsoidal fiber and the two other configurations. Arguably, the effective transverse coefficient of thermal expansion of composite with ellipsoidal fiber is lower than that for the composite with cylindrical and parallelepipedal fiber with a significate rate of difference.

Conclusion

To study the effect of geometrical configuration of fiber in the properties of homogenized composite material, numerical investigation of the micromechanical technique that leads to determine the effective mechanical properties and the coefficients of thermal expansions of unidirectional carbon-fiber/epoxy composites. However, three geometrical configurations of fiber are considered and the evolution of the effective properties with respect to the fiber volume fraction is shown and compared with each other. The main observations from this study are:

- Since the fiber is stiffer than the matrix, the greater the fiber's content the higher the stiffness of the composite and the lower of thermal expansion's coefficients.
- The effective mechanical properties, longitudinal and transversal Young's modulus as well as the effective shear modulus, are greater for the composites with ellipsoidal, i.e. a unidirectional carbon-fiber/epoxy composites with ellipsoidal fiber is more stiff than ones with cylindrical or parallelepipedal fibers.
- The configuration wherein the fiber has an ellipsoidal shape leads to lower effectives coefficients of thermal expansion, longitudinal and transversal, with a significant difference for the transversal modulus comparably to the composites with cylindrical or parallelepipedal fibers. Since the coefficients of thermal expansion depend on the bond strength between the atoms that make up the materials that' why the lower values of effectives coefficients of thermal expansion proves that the unidirectional carbon-fiber/epoxy composites with ellipsoidal fiber have strong bonds between atoms compared to the composites with cylindrical or parallelepipedal fibers.

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