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Evaluation of the effective viscoelastic properties of short fibers reinforced composites

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Abstract. In the present work, we address the calculation of the effective viscoelastic properties of short fibers reinforced composites via a semi-analytical approach that combines the two-scale Asymptotic Homogenization Method (AHM) and numerical computations based on Finite Elements (FE). As starting point and considering the elastic-viscoelastic correspondence principle, we propose the solution of the heterogeneous problem as a formal series expansion and then, we derive the associated local and homogenized problems along with the effective coefficients, all in the Laplace-Carson domain. Moreover, three-dimensional finite element simulations are performed to find the numerical solution of the local problems. Then, by inverting the Laplace-Carson transform, we obtain the effective coefficients in the time domain. We present the results for a viscoelastic composite reinforced by perfectly aligned short fibers. The influence of square or hexagonal periodic cells, as well as different fiber orientations, is analyzed. Finally, we deal with the case of random orientations.

Introduction

Innovative materials with improved mechanical properties are continuously demanded by high-performance applications in structural engineering. Fiber-reinforced composites are one of the most widely used and several examples consist of viscoelastic constituents in which their phases generally involve both instant elastic and time-dependent viscous behavior (see [1]). Short and discontinuous fibers usually act as fillers and, although the mechanical properties in terms of stiffness and strength of these composites are inferior to those reinforced with continuous fibers, the former are preferred in manufacturing processes due to the complexity associated with the use of long continuous fibers. For example, in injection molding, short fibers present a great advantage as allowing very short cycle times, which are mandatory in industries involving high volume [2].

The modeling of this kind of composites has been increasingly addressed in recent contributions. For instance, in [3], the Authors investigate the effective viscoelastic properties of short fiber-reinforced composites using Scott Blair-Rabotnov fractional-exponential operators. In [4], a variational model is proposed for the description of the failure mechanisms observed in short reinforcements subjected to tensile loading. Moreover, the Authors in [5] developed a micromechanics-based Artificial Neural Networks model to predict the elastic properties of short fiber composites.

The aim of this work is to calculate the effective viscoelastic properties of short fiber reinforced composite by means of a semi-analytical technique that combines the theoretical strengths of AHM with the advantages of developing three-dimensional finite element simulations. Specifically, AHM takes advantage of the well-separated length scales to decouple the spatial variables into a local and a global one. Thus, the analysis of the original problem at the macroscale is reduced to solving the local problems on the periodic cell [6]. Due to the lack of knowledge of an analytical solution, we perform a numerical approach based on the finite element method (FEM) providing a suitable alternative to

solve the local problems. For this purposes, we use the finite element software COMSOL Multiphysics[®] in conjunction with LiveLinkTM for Matlab[®] scripting.

It worth mentioning that we employ the modeling approach introduced in previous works **[7, 8]** and here we exploit it to perform the calculation in the case of short fiber reinforcements according to square or hexagonal arraignments, and different orientations. In addition, we investigate the effective coefficients for a particular case of random orientation.

Model Description and Statement of the Problem

Let us denote by $\Omega \subset \mathbb{R}^3$ a linear viscoelastic composite material with periodic microstructure and well-separated length scales ℓ and L. In particular, we consider Ω as a two-phase composite made of a viscoelastic matrix reinforced by square or hexagonal arrays of elastic short fibers (see Fig. 1). We define a dimensionless scaling parameter ε by the expression $\varepsilon = \frac{\ell}{L} \ll 1$. Additionally, in our

framework, x and y respectively refer to the macroscopic and the microscopic spatial variables, related through $y = \frac{x}{x}$.

In what follows, we consider the notation $\phi^{\varepsilon}(x,t) = \phi(x, y, t)$, where ϕ^{ε} is assumed to be periodic in *y*. Thus, since the constitutive response of all constituents is linear viscoelastic, ignoring inertia and external volume forces, the problem in Ω reads,

$$\nabla \cdot \boldsymbol{\sigma}^{\varepsilon}(x,t) = \mathbf{0} \qquad \text{in } (\Omega \setminus \Gamma^{\varepsilon}) \times \mathbb{R},$$

$$\left[\left[\boldsymbol{u}^{\varepsilon}(x,t) \right] \right] = \mathbf{0}, \qquad \left[\left[\boldsymbol{\sigma}^{\varepsilon}(x,t) \cdot \boldsymbol{n} \right] \right] = \mathbf{0}.$$
 (Eq.1)

As observed in Eq. 1, we further impose continuity conditions for displacements and tractions on $\Gamma^{\varepsilon} \times \mathbb{R}$. The term *n* stands for outward unit vectors to the surfaces Γ^{ε} and the operator $\llbracket \phi^{\varepsilon} \rrbracket$ denotes the jump of ϕ^{ε} across the interface between the constituents. More details about the boundary and initial conditions are reported in [7].

Regarding Eq. 1, the notation σ^{ε} represents the second-order stress tensor and the scale-dependent constitutive law for viscoelastic materials is stated,

$$\boldsymbol{\sigma}^{\varepsilon}(x,t) = \int_{0}^{t} \mathcal{R}^{\varepsilon}(x,t-\tau) : \frac{\partial \boldsymbol{\xi}(\boldsymbol{u}^{\varepsilon}(x,\tau))}{\partial \tau} d\tau.$$
(Eq.2)

Here, the term $\boldsymbol{u}^{\varepsilon}$ stands for the displacement field and the fourth-order tensor $\mathcal{R}^{\varepsilon}$ refers to the relaxation modulus, where the following symmetry properties are assumed $\mathcal{R}_{ijkl}^{\varepsilon} = \mathcal{R}_{ijkl}^{\varepsilon} = \mathcal{R}_{klij}^{\varepsilon}$. Additionally, $\boldsymbol{\xi}$ represents the second-order strain tensor and it is determined by the formula

$$\boldsymbol{\xi} \left(\boldsymbol{u}^{\varepsilon}(\boldsymbol{x},t) \right) = \frac{1}{2} \left(\nabla \ \boldsymbol{u}^{\varepsilon}(\boldsymbol{x},t) + \left(\nabla \ \boldsymbol{u}^{\varepsilon}(\boldsymbol{x},t) \right)^{T} \right).$$
(Eq.3)

Due to the scale-dependent constitutive law in Eq. 2 corresponds to the special form of a non-aging linear viscoelastic materials, we rely on the elastic-viscoelastic correspondence principle and the Laplace-Carson transform, and we rewrite Eq. 1 as follows,

$$\nabla \cdot \left[\hat{\mathcal{R}}^{\varepsilon} (x, s) : \boldsymbol{\xi} \left(\hat{\boldsymbol{u}}^{\varepsilon} (x, s) \right) \right] = \mathbf{0} \quad \text{in } (\Omega \setminus \Gamma^{\varepsilon}) \times [0, +\infty),$$

$$\left[\left[\hat{\boldsymbol{u}}^{\varepsilon} (x, s) \right] \right] = \mathbf{0}, \quad \left[\left[\left[\hat{\mathcal{R}}^{\varepsilon} (x, s) : \boldsymbol{\xi} \left(\hat{\boldsymbol{u}}^{\varepsilon} (x, s) \right) \right] \cdot \boldsymbol{n} \right] \right] = \mathbf{0}, \quad \text{on } \Gamma^{\varepsilon} \times [0, +\infty)$$
(Eq.4)

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Figure 1. The composite material is made up of a viscoelastic matrix reinforced by square or hexagonal arrangement of elastic short fibers with cylindrical shape. The fibers do not intersect the boundaries.

with the respective boundary and initial conditions. In Eq. 4, the "hat" symbol and variable s denote the Laplace-Carson domain.

Overview of the Semi-Analytical Approach

In this section, we present a brief description of the semi-analytical approach. For this purpose, we keep track of the methodology described in [7, 8] and highlight the main results of the asymptotic homogenization process and the required three-dimensional computational study.

The AHM [6] proposes the solution of the viscoelastic heterogeneous problem Eq. 4 as a formal series expansion in powers of ε , namely

$$\hat{\boldsymbol{u}}^{\varepsilon}(x,s) = \hat{\boldsymbol{u}}^{(0)}(x,y,s) + \sum_{i=1}^{+\infty} \hat{\boldsymbol{u}}^{(i)}(x,y,s)\varepsilon^{i}.$$
(Eq.5)

After substitution in Eq. 4, using the chain rule and equating the result in the same powers of ε , we obtain that, in the limit $\varepsilon \rightarrow 0$,

$$\hat{\boldsymbol{u}}^{(0)}(x,y,s) = \hat{\boldsymbol{v}}(x,s), \quad \hat{\boldsymbol{u}}_{m}^{(1)}(x,y,s) = \hat{\boldsymbol{\chi}}_{klm}(y,s)\boldsymbol{\xi}_{kl}\left(\hat{\boldsymbol{v}}(x,s)\right), \quad (\text{Eq.6})$$

where \hat{v} is a smooth vector function of x and s, and $\hat{\chi}_{klm}$ is a third order tensor periodic in y.

Moreover, by following the standard procedure, we derive the homogenized problems at the macroscale,

$$\hat{\mathcal{R}}_{ijkl}^{(*)}(s) \frac{\partial}{\partial x_{j}} \xi_{kl} \left(\hat{\boldsymbol{v}}(x,s) \right) = 0, \quad \Omega^{h} \times [0, +\infty)$$

$$\hat{\mathcal{R}}_{ijkl}^{(*)}(s) = \left\langle \hat{\mathcal{R}}_{ijkl}(y,s) + \hat{\mathcal{R}}_{ijpq}(y,s) \xi_{pq}^{(y)} \left(\hat{\boldsymbol{\chi}}_{kl}(y,s) \right) \right\rangle_{y},$$
(Eq.7)

with the respective boundary and initial conditions. The expression for the effective relaxation modulus, in Laplace-Carson space, is shown in Eq. 7.2, where the notation $\langle \cdot \rangle_y$ stands for the cell average operator. Furthermore, we have introduced the notation

$$\xi_{pq}^{(y)}\left(\hat{\boldsymbol{\chi}}_{kl}\left(y,s\right)\right) = \frac{1}{2} \left(\frac{\partial \hat{\boldsymbol{\chi}}_{klp}\left(y,s\right)}{\partial y_{q}} + \frac{\partial \hat{\boldsymbol{\chi}}_{klq}\left(y,s\right)}{\partial y_{p}}\right).$$
(Eq.8)

In addition, $\hat{\chi}_{klm}$ represents the solution of the local problems and a remarkable simplification emerges from assuming a *y*-constant nature of the relaxation modulus ($\hat{\mathcal{R}}_{ijkl}(y,s)$) along each phase in the periodic cell, namely

$$\hat{\mathcal{R}}_{ijkl}(y,s) = \begin{cases} \hat{\mathcal{R}}_{ijkl}^{(1)}(s), & \text{if } y \in Y_1 \\ \\ \hat{\mathcal{R}}_{ijkl}^{(2)}(s), & \text{if } y \in Y_2 \end{cases}$$
(Eq.9)

wherein superscripts (1), (2) indicate the corresponding constituents, i.e. the matrix and the inclusion. Considering the above, the local problems are stated,

$$\frac{\partial}{\partial y_{j}} \left[\hat{\mathcal{R}}_{ijpq}^{(\alpha)}(s) \xi_{pq}^{(y)}(\hat{\boldsymbol{\chi}}_{kl}^{(\alpha)}(y,s)) \right] = 0 \quad \text{in } Y_{\alpha} \times [0, +\infty) \quad (\alpha = 1, 2), \\
\hat{\boldsymbol{\chi}}_{klm}^{(1)}(y,s) = \hat{\boldsymbol{\chi}}_{klm}^{(2)}(y,s) \quad \text{on } \Gamma_{Y} \times [0, +\infty), \\
\left(\hat{\mathcal{R}}_{ijpq}^{(1)}(s) \xi_{pq}^{(y)}(\hat{\boldsymbol{\chi}}_{kl}^{(1)}(y,s)) \right) n_{j}^{(y)} - \left(\hat{\mathcal{R}}_{ijpq}^{(2)}(s) \xi_{pq}^{(y)}(\hat{\boldsymbol{\chi}}_{kl}^{(2)}(y,s)) \right) n_{j}^{(y)} = \hat{f}_{ikl}^{(y)}(s) \quad \text{on } \Gamma_{Y} \times [0, +\infty). \quad (\text{Eq.10})$$

Initial condition in $Y \times \{0\}$,

$$\hat{\chi}_{klm}(y,s) = 0$$

The interface loads $\hat{f}_{ikl}^{(y)}(s) := \left(\hat{\mathcal{R}}_{ijkl}^{(2)}(s) - \hat{\mathcal{R}}_{ijkl}^{(1)}(s)\right) n_j^{(y)}$ appear in the stress jump condition Eq. 10.3 and represent the driving force to obtain nontrivial solutions of the six elastic-type local problems $((k,l), k \ge l)$ when discontinuities in the coefficients Eq. 9, between the matrix and inclusions arise.

In summary, the semi-analytical technique (AHMFE) to calculate the effective viscoelastic properties consists, firstly, in numerically solving the set of elastic local problems Eq. 10 in Laplace-Carson space employing the finite element software COMSOL Multiphysics® and LiveLinkTM for Matlab® scripting. So that, we are able to calculate the effective relaxation modulus $\hat{\mathcal{R}}_{ijkl}^{(*)}(s)$ by means of Eq. 7.2. Finally, we applied the inversion of the Laplace-Carson transform to recover the original temporal space. We refer to Fig. 2 of [8] for more details about the methodology.

Results and Discussion

In this section, we study the two extreme cases that arise in the geometrical configurations of short fibers, i.e. perfectly aligned and random orientations.

The former is developed within the framework set up in section 5.2.3 of [8]. In particular, we consider a viscoelastic composite material with square or hexagonal arrangement of perfectly aligned short fibers (see Fig. 1). We deal with the pair T300 graphite fiber/ 934 epoxy matrix at room temperature. The properties of the transversely isotropic fibers are shown in Table 1 whereas the matrix is well modeled by the power-law

$$S_m(t) = \frac{1}{E_0} + Ct^n,$$
 (Eq.11)

and the properties for a constant bulk modulus are given in Table 2. In addition, we define the parameters $\gamma_1 := h_1 / H_1$ and $\gamma_2 := h_2 / H_2$ relating the measurement of fiber and matrix length in the square and hexagonal periodic cell, respectively (see Fig. 2 (d)).

$E_A^{(f)}$ [GPa]	$E_T^{(f)}$ [GPa]	$\mu_A^{(f)}$ [GPa]	$\mathcal{V}_A^{(f)}$	$V_T^{(f)}$
202.82	25.30	44.12	0.443	0.05

Table 1. Elastic moduli of the transversely isotropic fibers at room temperature.

The fibers are modeled as cylindrical and non-overlapped inclusions, centered in the periodic cell and which can uniformly rotate a counterclockwise angle θ about X_2 -axis for $0 \le \theta < \pi$.

$E_0^{(m)}$ [GPa]	$C^{(m)}\left[1/(\text{GPa} \times \min)\right]$	$n^{(m)}$	$K^{(m)}$ [GPa]
4.51	0.0135	0.17	3.9771

Table 2. Material properties of the viscoelastic matrix at room temperature.

In Fig. 2 (a), (b) and (c), we show the results for the effective moduli $E_1^{(*)}$, $\mu_{12}^{(*)}$ and $\nu_{32}^{(*)}$ for perfectly aligned short fibers, wherein the square and hexagonal periodic cells are highlighted in blue and black colors, respectively. We set a ratio γ as $\gamma = \gamma_1 = \gamma_2 = 3/5$ and a fiber volume fraction $V_f = 0.1$. In [8], we analyzed the rotation angles $\theta \in \{0^\circ, 90^\circ\}$. Here, however, we go further in our investigations and additionally consider $\theta \in \{10^\circ, 45^\circ\}$. The parameter study performed for θ reveals a new pattern in the results of $v_{32}^{(*)}$ in relation to what was observed in [8] and also confirm a decreasing behavior for $E_1^{(*)}$ and $\mu_{12}^{(*)}$. It should be noted that, by using a refined mesh, we obtain more accurate results than those shown in [8] for the hexagonal cell.

In regards to the random orientation case, we take inspiration from [9] and we model the randomness by means of a new periodic cell made of 27 similar short fibers embedded in the matrix. We consider all the 27 fibers to behave as T300 graphite and still use the 934 epoxy matrix. Now, by assuming a continuous uniform distribution in the interval $[0^\circ, 180^\circ]$ for the fiber orientations, we generate 27 random angles and rotate respectively each fiber about X_2 -axis. The frequency of occurrence is shown in the histogram of Fig. 2 (d). It is worth mentioning that as the inclusions are transversely isotropic, the relaxation modulus should be rotated according to each fiber orientation. In Fig. 2 (a), (b) and (c), we highlight in red color the effective moduli for the random orientation case.

Conclusions

In this work, we applied a semi-analytical approach to calculate the effective viscoelastic properties of short fiber reinforced composites. The model focused on three-dimensional geometrical configurations. We studied square and hexagonal fiber arrangements along with different fiber orientations. In addition, the fiber orientation analysis comprised two different cases, namely perfectly aligned and randomly oriented. The results indicated that these geometrical features influence the macroscopic effective response of the viscoelastic composite.

A further generalization of the present framework includes the consideration of fiber orientations with two degrees of freedom allowing us to achieve any orientation in three-dimensional space. Another extension could be to take into account different aspect ratios of the fibers.



Figure 2. Chart (a), (b) and (c) shows the calculation of the effective moduli. Chart (d) offers general information.

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