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A hybrid method for computing the effective properties of composites containing arbitrarily shaped inclusions

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ABSTRACT

A novel hybrid method is developed to compute the effective properties of composites containing arbitrarily shaped inclusions. In this method, finite element analysis of a single inclusion representative volume element model is used to compute the Eshelby tensor of the inclusion. This tensor is substituted into Mori–Tanaka model to compute the effective properties. Predictions by the hybrid method are compared with the predictions by a pure analytical method as well as a pure numerical method. Results indicate that the composites with triangular, rectangular and irregular section inclusions have significantly better effective properties than the corresponding composites with circular section inclusions.

1. Introduction

In order to achieve weight reduction, composite materials are extensively used in many aerospace and automotive applications. Effective properties of these materials depend on microstructural parameters such as constituent material properties, inclusion volume fraction (V_f), inclusion spatial arrangement, inclusion orientation, inclusion coating and inclusion shape. Present study focuses on the influence of inclusion shape on the effective properties of composite materials.

Kim and Park [1] and Park et al. [2] experimentally investigated the effective properties of C-section carbon fiber reinforced cementitious composites; and their results indicated that these composites have better mechanical properties than the composites reinforced with circular section (i.e. cylindrical) carbon fibers. Experimental investigation by Xu et al. [3] showed that the composites with kidney section carbon fibers had better interfacial shear strength and interlaminar shear strength compared to those with circular section carbon fibers. Liu et al. [4] have performed experiments on the composites with triangular section carbon fibers. They have shown that these composites have better flexural strength and flexural modulus than those with circular section carbon fibers. Zhu and Beyerlein [5] have shown that the bone-shaped short fiber reinforced composites have more strength and toughness compared to the conventional short straight fiber reinforced composites. Finite element (FE) analysis was used by Zhou et al. [6] to obtain the optimum fiber shape that gives maximum stiffness to the composite. From these studies, it is clear that the fiber shape has a significant influence on the effective properties of composites.

Many analytical methods [7–12] are available for computing the effective properties of unidirectional (UD) composite materials. Most of these methods are based on the concept of Eshelby tensor [13]. The dilute Eshelby model [8] is accurate in predicting the effective properties of composites with very low fiber volume fraction. However, this method is not suitable for non-dilute composites. Effective properties of the non-dilute composites can be computed by using analytical models such as the Mori–Tanaka (MT) model [9,10], self-consistent model [11] and bounding models [12]. The main limitation of these analytical methods is that analytical expressions for the Eshelby tensor are available only for ellipsoidal [14] and polyhedral inclusions [15]. Therefore, in these analytical methods, actual inclusions are replaced by equivalent ellipsoidal inclusions with appropriately selected aspect ratios. In the case of inclusions with complicated geometry, different ellipsoidal inclusions are combined together to represent a single inclusion [16,17]. In many cases, the equivalent ellipsoidal inclusion may not accurately capture the effect of actual inclusion shape on the effective properties. For example, replacing a circular section inclusion with an equivalent ellipsoidal inclusion can lead

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to an error in the prediction of effective properties of composites with high material property mismatch ratios [18].

Effective properties of composites can also be computed through pure FE based numerical micromechanical approaches [19–27]. Kari et al. [19] and Pan et al. [20] have used the FE based approach to compute the effective properties of discontinuous fiber reinforced (DFR) composites. "ArtiComp" program was developed by Srinivasulu et al. [21] to compute the effective properties of DFR composites with straight fibers and curved fibers. Hine et al. [22] have used Monte-Carlo procedures to compute the effective properties of DFR composites. Mishnaevsky [23] has developed the "Meso3D" program to compute the effective properties of particle reinforced composites. "Nanocomp 3D" program was developed by Wang et al. [24] to compute the effective properties of nanocomposites. Zohdi [25] studied composite materials containing randomly oriented block-like and spherical shaped particulate reinforcements. A computational method was developed to determine optimal geometrical parameters and mechanical properties of particulate reinforcements to achieve the desired effective properties. In order to resolve the difficulties involved in the optimization process, a statistical genetic algorithm was also developed [26]. The pure FE based numerical approach is generic in nature; there is no limitation on the inclusion shape. However, this method is computationally expensive because a new FE analysis has to be performed for every change in the microstructural parameters of the composite. Therefore, although the pure numerical approach is capable of computing the effective properties of the composites with arbitrarily shaped inclusions, this approach demands for extensive computational resources. Therefore, there is a need for a more efficient method to compute the effective properties of the composites with arbitrarily shaped inclusions.

In this study, a novel hybrid method is proposed to compute the effective properties of composites with arbitrarily shaped inclusions. In this method, Eshelby tensors of arbitrarily shaped inclusion are computed through the FE based numerical approach. This FE based Eshelby tensor is then substituted into the MT analytical model to compute the effective properties. This method is computationally more efficient than the pure numerical approach. The hybrid method is used to compute the effective properties of composites reinforced with arbitrarily shaped inclusions such as prolate spheroidal, oblate spheroidal, circular section, triangular section, rectangular section and irregular section inclusions. The results illustrate the influence of inclusion shape on the effective properties of composites. For comparison purpose, the effective properties computed by using the pure analytical method and the pure numerical method are also presented.

2. Hybrid method

In the hybrid method, the equivalent Eshelby tensor (ξ^{HYB}) of an arbitrarily shaped inclusion is computed through the FE based micromechanics approach. Six inclusion shapes: prolate spheroidal, oblate spheroidal, circular section, triangular section, rectangular section and irregular section inclusions are considered (Fig. 1). In this method, a large cubic representative volume element (RVE) model of a composite material containing a single inclusion is generated. Homogeneous Boundary Conditions (HBCs) [28] are applied on the boundary surfaces of the RVE model. HBCs are obtained from Eq. (1),

$$\int_{\partial V} (t_i - \bar{\sigma}_{ij} n_j)(u_i - \bar{\varepsilon}_{ij} x_j) d\Omega = 0 \tag{1}$$

In the above equation, ∂V represents the boundary surfaces of RVE, t_i is the traction, u_i is the displacement, x_j is the position, n_j is the surface normal, $\bar{\varepsilon}_{ij}$ is the average strain and $\bar{\sigma}_{ij}$ is the average stress.

Three extensional and three shear deformation load cases are used in this analysis. The first load case represents extension loading in longitudinal direction. In this load case, only $\varepsilon_{11} = \varepsilon_{11}^{app}$ is nonzero. ε_{11}^{app} represents the applied strain in longitudinal direction. HBCs for this load case are as follows,

$$\begin{Bmatrix} u_1 \\ u_2 \\ u_3 \end{Bmatrix} = \begin{bmatrix} \varepsilon_{11}^{app} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} \varepsilon_{11}^{app} x_1 \\ 0 \\ 0 \end{Bmatrix} \tag{2}$$

This implies,

$$u_1 = \varepsilon_{11}^{app} x_1; \quad u_2 = 0 \ \& \ u_3 = 0 \tag{3}$$

FE analysis is performed by using ABAQUS/standard implicit solver [29] to obtain the stress and strain distributions inside the RVE model. Eq. (4) is used to obtain the average strain ($\bar{\varepsilon}_{ij}^f$) in the inclusion.

$$\bar{\varepsilon}_{ij}^f = \frac{1}{V^f} \int \varepsilon_{ij}^f dV = \frac{\sum_{e=1}^{NE} \left(\varepsilon_{ij}^f dV \right)_e}{\sum_{e=1}^{NE} (dV)_e} \tag{4}$$

In the above equation, V^f represents the inclusion volume, ε_{ij}^f represents the strain in inclusion, NE represents the number of elements in inclusion and dV represents the element volume.

The average strain in the composite ($\bar{\varepsilon}$) and average strain in the inclusion ($\bar{\varepsilon}^f$) are related to each other through strain concentration tensor (A^{HYB}) as,

$$\bar{\varepsilon}^f = A^{HYB} \bar{\varepsilon} \tag{5}$$

From the first load case, components of A^{HYB} are computed as,

$$A_{11}^{HYB} = \frac{\bar{\varepsilon}_{11}^f}{\varepsilon_{11}^{app}}, A_{21}^{HYB} = \frac{\bar{\varepsilon}_{22}^f}{\varepsilon_{11}^{app}}, A_{31}^{HYB} = \frac{\bar{\varepsilon}_{33}^f}{\varepsilon_{11}^{app}}, A_{41}^{HYB} = \frac{\bar{\varepsilon}_{23}^f}{\varepsilon_{11}^{app}},$$
$$A_{51}^{HYB} = \frac{\bar{\varepsilon}_{13}^f}{\varepsilon_{11}^{app}} \ \& \ A_{61}^{HYB} = \frac{\bar{\varepsilon}_{12}^f}{\varepsilon_{11}^{app}} \tag{6}$$

Other components of A^{HYB} are computed from the remaining five load cases. The strain concentration tensor of a dilute composite can also be analytically computed through the dilute Eshelby model [8].

$$A^{dil} = [I + \xi C_m^{-1}(C_f - C_m)]^{-1} \tag{7}$$

In the above equation, C_m and C_f represent elastic stiffness tensor of matrix and inclusion materials respectively and I represents a fourth order identity tensor. By replacing A^{dil} in Eq. (7) with A^{HYB}, the FE based Eshelby tensor (ξ^{HYB}) is obtained as,

$$\xi^{HYB} = (A^{HYB^{-1}} - I)(C_m^{-1} C_f - I)^{-1} \tag{8}$$

In contrast to analytical methods, computation of ξ^{HYB} through the FE based approach is not limited by the inclusion shape. After computing ξ^{HYB}, it is substituted into the MT analytical model [9,10] to compute the effective properties of non-dilute UD DFR composites with arbitrarily shaped inclusions. As per the MT method, elastic stiffness tensor (C^{MT}) of a UD DFR composite is given by,

$$C^{MT} = \left(V_m C_m + \sum_{f=1}^{n} V_f C_f \left[I + \xi^{HYB} C_m^{-1}(C_f - C_m) \right]^{-1} \right)$$
$$\times \left(V_m I + \sum_{f=1}^{n} V_f \left[I + \xi^{HYB} C_m^{-1}(C_f - C_m) \right]^{-1} \right)^{-1} \tag{9}$$

In the above equation, V_m and V_f represent volume fractions of matrix and inclusions respectively. Summation indicates that the inclusions can be of different shapes. Finally, the effective elastic material properties are computed from C^{MT}.