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Effective thermal conductivity of composite ellipsoid assemblages with weakly conducting interfaces

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ABSTRACT

In this work, a coated ellipsoid assemblage model for the prediction of the effective thermal conductivity of composites with imperfect interfaces is developed. Based on the Green's function technique, the study proposes a new formulation of the composite ellipsoid assemblage model with an imperfect interface between the inclusion and the surrounding matrix. The solution of the integral equation is obtained thanks to the concept of interior- and exterior-point Eshelby's conduction tensors. Thereafter, the analytical expressions of the heat intensity and the effective thermal conductivity are proposed for ellipsoidal inclusion and anisotropic thermal conductivity per local phase. In order to test the relevance of the model, its predictions have been compared with the exact solutions of spherical and cylindrical inclusion. Moreover, the capability of the model to well describe the thermal behaviour of composites with high volume fractions of inclusions has been tested through some comparisons with numerical results proposed in the literature. A parametric study is then conducted to analyse the effects of the morphology and the volume fraction of the inclusion, the interface thermal resistance and contrast of thermal conductivity of local phases, on the predictions of the developed model.

1. Introduction

During the last decades, the use of composite materials became more widespread in industrial sectors such as aeronautics, automotive, transport electronics, etc. The main advantage of this kind of materials is their ability to adapt their properties to specific applications. The resulting properties of the composite strongly depend on the microstructure and the properties of its constituents. The composites consist of one or more discontinuous phases (inclusions) dispersed in a continuous phase (matrix). The prediction of the properties of these heterogeneous materials is of great interest for the design of new composites.

In the field of transfer phenomena in heterogeneous materials, the thermal conductivity analysis is of great interest in the design of new composites in modern engineering applications such as electronic packaging, thermal insulation, etc. The optimization of the thermal conductivity is a key step in the design and development of these composites. The homogenization methods based on multi-scale modeling are tailoring tools for the determination of the effective properties of the composite from the morphology, the volume fraction, the orientations and the properties of each local phase. The interfaces between the constituents play a key role during the transfer phenomena such as the thermal conductivity, electrical conductivity, diffusivity, permeability, etc. The modeling of thermal conductivity of composite materials has been widely studied and reported in the literature. Most of these approaches are conducted under the main assumption of perfect interfaces between local constituents of the composite. However, in some situations these interfaces are imperfect due to the poor chemical adhesion, the presence of a relative roughness and a difference of the thermal expansion between the local phases. These imperfections can induce an interfacial thermal resistance that results in a jump of the temperature field at the interfaces and greatly affects the thermal transfer in the composite. According to the Kapitza interfacial thermal resistance model [1], this temperature jump is assumed proportional to the normal component of the heat flux. Some investigations have been devoted to the determination of the effective conductivity of heterogeneous materials with imperfect interfaces. Developed within the framework of the mean fields homogenization methods, these initial studies reported in the literature can be classified into three categories.

The first class of models results from the solution of the problem of the Eshelby's inclusion embedded in an infinite matrix. This solution was initially developed in elasticity by Eshelby [2] and then reformulated in thermal conductivity by Hatta and Taya [3–4] and in the presence of an interfacial thermal resistance between the inclusions and

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the matrix by Le Quang et al. [5] and Bonfoh et al. [6]. However, these models appear not relevant in the case of voids, high volume fractions and rigid inclusions [7].

The second class of models is based on the concept of inclusion surrounded by a matrix called 'coated inclusion' or 'composite inclusion'. Two approaches have been then developed within this second class. The first one deals with the composite sphere assemblage (CSA) that considers two concentric spheres [8]. The second one is related to the generalized self-consistent (GSC) approach initially suggested by Christensen and Lo [9]; Christensen [10]. In [9–10], the analysis showed that these models based on the concept of coated inclusion provide results in good agreement with numerical simulations and experimental data of effective properties, even for moderated volume fractions and for rigid inclusions. In the case of the thermal conductivity, the initial investigation dealing with the modeling of the effective thermal conductivity of heterogeneous materials is based on the well-known work of Maxwell [11] and Rayleigh [12]. These authors provide the solution of the Laplace's equation describing the heat transfer in the case of an isotropic thermal conductivity per phase. Maxwell [11] suggested an approach to model the thermal conductivity of a composite with small concentration of spherical inclusions. Hashin and Shtrikman [13] proposed the famous lower and upper bounds of the thermal conductivity of a macroscopically isotropic two-phase material. In this context, Hashin [14] determined the thermal conductivity of an isotropic two-phase material in the framework of the generalized self-consistent scheme (GSCS). These models were developed under the hypothesis of a perfect interface between the constituents of the composite. Hasselman and Johnson [15] modified the approach suggested by Maxwell [11] and Rayleigh [12] to account for the interfacial thermal resistance for composites containing spherical or cylindrical inclusions. In the case of ellipsoidal inclusions, the solution of the Laplace's equation can be expressed in terms of ellipsoidal harmonic functions and through the theory of potentials defined in ellipsoidal coordinates by Kellog [16].

The CSA model has been extended to ellipsoidal inclusions through the composite ellipsoids assemblage (CEA). Dealing with thermal conductivity behavior, Hatta and Taya [17] suggested the solution of the problem of coated spheroidal inclusion embedded in an infinite matrix. By considering non-dilute concentrations of ellipsoidal voids or inclusions, Benveniste and Miloh [18]; Miloh and Benveniste [19] proposed the exact solution based on the CEA model. Giordano [20] then adapted the solution of coated inclusion for the modeling of the non-linear behavior of three phases composite with coated inclusions. Thanks to a linear transformation of Cartesian coordinates, Milton [21] provided the exact expressions of the effective conductivity of the CEA model in the case of anisotropic thermal conductivity.

The third type of models deals with the concept of an interphase located between the inclusion and the matrix. Then, the models of imperfect interfaces are deduced when the thickness of the interphase tends asymptotically to zero and its conductivity to infinity for highly conducting interfaces. The weakly conducting interfaces case is also deduced from the interphase problem by tending both the thickness and the conductivity of the interphase to zero [22–26].

To our knowledge, the application of the CEA model to imperfect interfaces between the constituents of a composite is not reported in the literature. The analytical modeling of the thermal conductivity of the composite inclusion in the presence of an imperfect interface surrounding the ellipsoid remains new challenge in the field of homogenization of composites.

The present study proposes a composite ellipsoid assemblage model with imperfect interface in order to provide an accurate model for composite with ellipsoidal inclusion and anisotropic thermal conductivity per phase. Unlike models providing the solution the Laplace's equation in terms of ellipsoidal harmonics, we propose a new micromechanical formulation of the CEA model based on the Green's function technique and the integral equation. The obtained integral relation displays a surface integral related to the temperature jump at the imperfect interface. The exact calculation of this surface integral is difficult. Thus, in the present model the local heat flux on this imperfect interface is approximated by its volume average inside the corresponding inclusion.

The manuscript is organized as following: the Section 2 is devoted to the description of the micromechanical approach proposed for the problem of heterogeneous anisotropic material containing ellipsoidal inclusions with an interfacial thermal resistance. Afterwards, the obtained localization equation enables to determine the effective thermal conductivity of the composite in Section 3. In Section 4, some comparisons with results of previous investigations within both isotropic and anisotropic configurations are then performed in order to examine the relevance of the elaborated approach. Finally, the aspect ratio, the volume fraction of inclusions, the local contrast of thermal conductivities, the anisotropy of matrix's phase and the interface parameter, dependent effective conductivity of reinforced composites are investigated and discussed in details.

2. Micromechanical modeling

We consider a representative volume element (RVE) with volume V of the composite that consists of ellipsoidal inclusions embedded in a homogeneous matrix. Let $\boldsymbol{q}(\boldsymbol{r})$, $\boldsymbol{e}(\boldsymbol{r})$ and $T(\boldsymbol{r})$, denote respectively the heat flux, the intensity and the temperature fields at the vector position $\boldsymbol{r}(x_1, x_2, x_3)$ in the RVE. The thermal behavior of the composite is assumed linear and described by its local thermal conductivity tensor $\boldsymbol{k}(\boldsymbol{r})$. The RVE is subjected to a homogeneous intensity field $\boldsymbol{e}^0$ at its boundary ∂V. The present study deals with the determination of the intensity field $\boldsymbol{e}(\boldsymbol{r})$ and the heat flux $\boldsymbol{q}(\boldsymbol{r})$ as well as the prediction of the effective thermal conductivity of the composite.

2.1. Basic equations

Under steady-state conditions and in absence of internal thermal source, the field equations of the heterogeneous thermal conductivity problem read:

- the linear thermal behavior described by Fourier's law

$$\boldsymbol{q}(\boldsymbol{r}) = \boldsymbol{k}(\boldsymbol{r}).\ \boldsymbol{e}(\boldsymbol{r}) \tag{1}$$

- the energy conservation equation

$$\boldsymbol{div}\ \boldsymbol{q}(\boldsymbol{r}) = 0 \tag{2}$$

- the intensity field

$$\boldsymbol{e}(\boldsymbol{r}) = -\nabla T(\boldsymbol{r}) \tag{3}$$

- the boundary conditions

$$T(\boldsymbol{r}) = -\boldsymbol{e}^0.\ \boldsymbol{r} \quad for\ \boldsymbol{r} \in \partial V \tag{4}$$

Within the present study, the interfaces S between the inclusions and the matrix are assumed imperfect so that:

$$\begin{aligned} &[T(\boldsymbol{r})] = T^+(\boldsymbol{r}) - T^-(\boldsymbol{r}) \neq 0 \\ &[\boldsymbol{q}(\boldsymbol{r})].\ \boldsymbol{n} = (\boldsymbol{q}^+(\boldsymbol{r}) - \boldsymbol{q}^-(\boldsymbol{r})).\ \boldsymbol{n} = 0 \quad \text{for } \boldsymbol{r} \in S \end{aligned} \tag{5}$$

where $\boldsymbol{n}$ is the unit vector normal to S oriented from S^- to S^+; $T^+(\boldsymbol{r})$ and $\boldsymbol{q}^+(\boldsymbol{r})$ (respectively $T^-(\boldsymbol{r})$ and $\boldsymbol{q}^-(\boldsymbol{r})$) are the fields defined on the face S^+ (respectively S^-).

2.2. Integral equation for a heterogeneous finite medium

We consider a finite homogeneous reference medium (HRM) with the thermal conductivity $\boldsymbol{k}^0$ so that the local thermal conductivity