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Anisotropic thermal conductivity of composites with ellipsoidal inclusions and highly conducting interfaces

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ABSTRACT

The present paper deals with the micromechanical modeling of the effective thermal conductivity of composite materials containing ellipsoidal inclusions with highly conducting interfaces. At these interfaces between inclusions and the surrounding medium, the temperature field is assumed continuous while the heat flux undergoes to a discontinuity. The proposed model is based on the solution of the Eshelby's inclusion problem with highly conducting interfaces. Moreover, the present study is conducted in the general case of an anisotropic thermal conductivity per phase and ellipsoidal inclusions.

Results in terms of the thermal intensity field inside each phase are proposed and then analyzed in light of the effects of some model parameters. The effective thermal conductivity of the composite has been predicted through classical homogenization schemes such as the Dilute medium, the Mori-Tanaka and the Differential schemes. The model predictions have been also compared with some results provided by previous investigations.

1. Introduction

For the determination of the effective thermal conductivity of composites, the classical homogenization methods assume perfect interfaces between the inclusions and the matrix. In reality, these interfaces are imperfects and involve a discontinuity of the temperature or the normal heat flux. In such a situation, two cases are distinguished.

The first one deals with imperfect interfaces exhibiting the discontinuity of the temperature while the normal heat flux remains continuous. These interfaces known as weakly conducting or low conducting (LC) interfaces [1] are essentially due to the roughness, the poor mechanical or chemical adhesion, the presence of a thin layer of low thermal conductivity inserted between the local phases of the composite [2]. These imperfect interfaces reduce the effective thermal conductivity of the composite. The problem of the thermal conductivity in composite with LC interfaces has been the subject of some investigations in recent years [3–9].

The second case of imperfect interfaces induces the discontinuity of the normal heat flux, while the temperature remains continuous. This phenomenon appears mainly in the case of a thin interphase of high thermal conductivity located between the constituents of the composite. The passage from a highly conducting interphase to an imperfect interface has been rigorously established by Pham Huy and Sanchez-Palencia [10].

In the literature, some works have been devoted to the modelling of composite with highly conducting (HC) interfaces:

The first type is based on the Hashin-Shtrikman variational principles and aims to evaluate the lower and upper bounds of the effective conductivity of heterogeneous materials [5,11,12]. These variational methods provide explicit expressions of the upper and lower bounds of the conductivity of two-phase composites containing spherical inclusions.

The second type concerns some numerical methods for the determination of the effective conductivity of composites with HC interfaces. For example, by combining the level-set method and the extended finite element method, the Fourier transform method is applied to periodic composites [13,14].

The third type deals with the concept of highly conducting interphase located between the inclusions and the matrix. Then, models of imperfect interfaces are deduced asymptotically when the thickness of the interphase tends to zero and the conductivity of the interphase to infinity [15–19].

The fourth one is based on the Fourier's law governing the heat transfer. The solution of the corresponding heat equation has been initially suggested by Rayleigh [20] and Maxwell [21], thanks to spherical harmonic functions. Then, Cheng and Torquato [7]

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Nomenclature

T	temperature (K)
x_1, x_2, x_3	cartesian coordinates
a_1, a_2, a_3	semi-axis of the ellipsoidal inclusion
f	volume fraction of inclusions
S_I	interface between inclusions and matrix (m^2)
g	Green's function
V	volume of the representative volume element RVE (m^3)
V_I	volume of inclusions (m^3)
∂V	boundary of the considered RVE (m^2)
$\boldsymbol{r}$	vector position of the current point
$\boldsymbol{e}$	local intensity field ($K{\cdot}m^{-1}$)
$\boldsymbol{E}$	macroscopic intensity field ($K{\cdot}m^{-1}$)
$\boldsymbol{q}$	local heat flux ($W{\cdot}m^{-2}$)
$\boldsymbol{Q}$	macroscopic heat flux ($W{\cdot}m^{-2}$)
$\boldsymbol{n}$	outward unit vector normal to the interface S
$\boldsymbol{N}$	outward unit vector normal to the boundary ∂V
$\boldsymbol{k}$	tensor of thermal conductivity ($W{\cdot}m^{-1}{\cdot}K^{-1}$)
$\boldsymbol{k}^I$	tensor of thermal conductivity of inclusions ($W{\cdot}m^{-1}{\cdot}K^{-1}$)
$\boldsymbol{k}^M$	tensor of thermal conductivity of the matrix ($W{\cdot}m^{-1}{\cdot}K^{-1}$)
$\boldsymbol{k}^{eff}$	tensor of effective thermal conductivity of the composite ($W{\cdot}m^{-1}{\cdot}K^{-1}$)
$\boldsymbol{h} = \boldsymbol{k}^{-1}$	tensor of thermal resistivity ($m{\cdot}K{\cdot}W^{-1}$)
$\boldsymbol{\Lambda}$	Green's vector
$\boldsymbol{G}^I$	interior-point Eshelby's thermal conduction vector
$\boldsymbol{G}^E$	exterior-point Eshelby's thermal conduction vector
$\boldsymbol{\Gamma}$	modified Green's tensor
$\boldsymbol{S}^I$	interior-point Eshelby's thermal conduction tensor

Greek symbols

$\delta(\boldsymbol{r})$	Dirac function
δ_{ij}	Kronecker delta
α	interface thermal parameter ($W{\cdot}K^{-1}$)
$\nabla T(\boldsymbol{r})$	temperature gradient: $\nabla_i T(\boldsymbol{r}) = \partial T(\boldsymbol{r})/x_i$

extended this method to periodic composites with HC interfaces. Theses previous investigations provide analytical expressions of the effective thermal conductivity, but are restricted to particular cases of spherical or cylindrical inclusions and isotropic thermal conductivity per phase. Miloh and Benveniste [22] generalized this method to spheroidal inclusions by expressing the solution of the Laplace's equation in terms of ellipsoidal harmonic functions. These authors also restricted themselves to the case of isotropic thermal conductivity.

In light of these previous investigations, the solution of the problem of thermal conductivity in composites with HC interfaces, in the general case of ellipsoidal inclusions and anisotropic thermal conductivity per phase remains a challenge. The present study suggests a micromechanical model to treat this general case.

Based on the Green's function technique, we propose the solution of this problem of heterogeneous thermal conductivity in the framework of the Eshelby's inclusion model. This approach has been investigated by Le Quang et al. [23] in the particular case of spherical inclusions. In the present study, we propose a new formulation based on the interior- and exterior-point Eshelby's conduction tensors for the problem of an ellipsoidal inclusion embedded in a matrix with HC interfaces. Moreover, contrary to initial investigations, the thermal conductivity is assumed anisotropic per phase.

The present manuscript is organized as follows. The Section 2 develops the general micromechanical approach. Afterwards, classical homogenization schemes are elaborated to evaluate the effective thermal conductivity of composites in Section 3. In Section 4, some simulations are conducted in order to derive the effective thermal conductivity within both anisotropic and isotropic configurations. Comparisons with results of previous investigations are also 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 and the interface parameter, dependent effective conductivity of composites are investigated and discussed in details.

2. Micromechanical model

The representative volume element (RVE) with volume V of the composite material 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 $\boldsymbol{r}(x_1, x_2, x_3)$ of the RVE. The thermal behaviour of the composite is linear and described by the 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, in one hand, with the determination of the local intensity field $\boldsymbol{e}(\boldsymbol{r})$ and the heat flux $\boldsymbol{q}(\boldsymbol{r})$. On the other hand, the present investigation aims to predict the effective thermal conductivity of composite materials.

2.1. Basic equations

Under steady-state conditions and in the absence of internal thermal source, the field equations of of such an heterogeneous thermal conductivity problem are defined by the:

- Linear thermal behaviour described by Fourier's law

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

- Energy conservation equation

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

- Intensity field

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

- Boundary conditions

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

Within the present study, the interfaces S between inclusions and the matrix are assumed highly conducting (HC):

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

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 S^+ (respectively S^-).

2.2. Integral equation

The local thermal conductivity tensor $\boldsymbol{k}(\boldsymbol{r})$ can be split into a uniform part $\boldsymbol{k}^0$ of the homogeneous reference medium (HRM) and a fluctuating one $\delta\boldsymbol{k}(\boldsymbol{r})$: