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Closed-form estimates for the effective conductivity of isotropic composites with spherical particles and general imperfect interfaces

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ABSTRACT

The present paper is concerned with estimating the effective conductivity of a composite consisting of spherical particles dispersed inside a matrix in a statistically homogeneous and isotropic way. The interface between every spherical particle and the matrix is thermally imperfect and described by the general linear isotropic imperfect model resulting from the replacement of an interphase of weak thickness by an interface of zero thickness. This general model includes as extreme particular cases Kapitza's (or lowly conducting) thermal resistance model and the highly conducting thermal imperfect interface model. The fundamental solution is derived for the problem of a spherical particle embedded, via a general imperfect interface, in an infinite matrix undergoing a remote uniform intensity boundary loading. With the help of this fundamental solution, closed-form estimates for the size-dependent effective conductivity of the composite are deduced by using the dilute distribution, Mori–Tanaka, self-consistent and generalized self-consistent schemes. These results, incorporating as particular ones all the relevant estimates reported in the literature, are discussed and compared through numerical examples.

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1. Introduction

The study of interface effects in composites is a research subject of lasting interest (see, e.g., [1–6]). This is, in particular, because in many practical situations, the interfaces between the constituent phases of a composite are often imperfect and strongly affect its effective properties. In the context of linear thermal conduction, there are mainly three models proposed for modeling imperfect interfaces (see, e.g., [7–14]). The first one is the well-known Kapitza's thermal resistance or lowly conducting (LC) interface model. According to this model, the temperature suffers a jump an interface while the normal heat flux is continuous across it and proportional to the temperature jump. The second one is the highly conducting (HC) interface model in which the temperature is continuous across an interface while the normal heat flux across the same interface is discontinuous and has to verify the Laplace-Young equation. The third one is the general interface model which is proposed by Benveniste [15], Bövik [16] and Gu and He [17] on the basis of the replacement of a thin interphase by an imperfect interface. This model is characterized by two relations governing the temperature and normal heat flux jumps. Moreover, the general imperfect interface model includes the LC and HC interface models as particular cases. Indeed, upon requiring the conductivity of the interphase to be much lower or higher than that of each of its surrounding phases, the two latter ones can be retrieved from the former one [15,10].

Significant progress has been accomplished in studying the effects of imperfect interfaces on the effective conductivity of composites by theoretical analysis (see, e.g., [3,7,9,23,12,18–22]), by numerical simulations (see, e.g., [24–27]), or by experimental efforts (see, e.g., [14,21,28,29]). Concerning theoretical analysis, the works [23,30], for example, analyzed the effect of the LC and HC interfaces by using the equivalent inhomogeneity method in which an equivalent inhomogeneity perfectly bonded to the infinite matrix is used to replace an imperfectly bonded inhomogeneity in an infinite matrix under an energy equivalency condition; in the paper [8], closed-form estimates have been derived for the effective conductivity of a composite in which spheroidal inhomogeneities are embedded via LC interfaces; in [18,19], Le Quand et al. provided closed-form estimates for the effective anisotropic

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conductivity of composite with LC and HC interfaces by using the extended Eshelby tensors; in [31,32], Lipton and Talbot established the upper and lower bounds on the effective conductivity of composites with LC and HC interfaces by using appropriate variational principles. In regard to numerical simulations, Yvonnet et al. [26,27] simulated the LC and HC interface effects by combining the level-set method (LSM) and the extended finite element method (XFEM); Dolbow et al. [24,25] proposed a finite element method based on the Nitsche technique to deal with a transport problem in which the temperature and normal flux discontinuities intervene. In the framework of experimental research, some authors [22,29] determined the HC interface material parameters in a composite by using inverse analysis. However, the works reported in the literature on the linear imperfect interfaces in composites are almost exclusively limited to either the LC or HC interface. Consequently, the study of the effects of general linear imperfect interfaces on the effective thermal conductivity of composites remains a largely open research issue.

The present work is concerned with micromechanical estimation of the effective conductivity of composites consisting of a matrix in which spherical inhomogeneities are embedded via general imperfect interfaces. It has the following two objectives:

1. First, it aims at deriving the solution to the important auxiliary problem of a spherical particle in an infinite matrix via an imperfect interface. This solution of general importance can in particular be applied to establish the relations between the local and global fields. In contrast with the relevant results reported in the literature (see, e.g., [8,18,19]), which often hold only for the LC or HC interface, our results are valid for the general linear imperfect interface.
2. Second, it has the purpose of estimating the effective conductivity of composites in question by adjusting the well-established micromechanical schemes to the presence of general imperfect interfaces in them. This purpose will be achieved by using the solution derived for the auxiliary problem, by choosing an appropriate reference phase and by imposing relevant boundary conditions according as the micromechanical scheme is applied. In particular, we show that our results include as particular ones those obtained in [8,18,19] for the LC and HC interfaces.

The paper is organized as follows. In the next section, the background of the problem to be solved is presented with emphasis on the general linear isotropic thermal imperfect interface model and its relations to Kapitza's (or LC) and HC interface models. Section 3 is dedicated to deriving the fundamental solution to the problem of a spherical inhomogeneity embedded via a general linear isotropic imperfect interface in an infinite matrix undergoing a remote uniform intensity loading. In Section 4, with help of the fundamental solution obtained in Section 3, the closed-form estimates are deduced for the effective conductivity of isotropic composites in question by successively using the dilute distribution, Mori–Tanaka, self-consistent and generalized self-consistent schemes. In Section 5, numerical examples are provided to illustrate the results of Section 4 and, in particular, the size-dependency of the effective conductivity. In Section 6, a few concluding remarks are drawn.

2. Setting of the problem

The composite under consideration consists of m spherical inhomogeneities embedded in a matrix. Let Ω be the three-dimensional (3D) domain bounded by $\partial\Omega$ and occupied by a representative volume element (RVE) of the composite. The subdomains of Ω occupied by the matrix and the ith inhomogeneity (or inclusion) are designated by $\Omega^{(M)}$ and $\Omega^{(i)}$ such that $\Omega = \Omega^{(M)} \cup \Omega^{(1)} \cup \cdots \cup \Omega^{(m-1)} \cup \Omega^{(m)}$. The interface between the matrix $\Omega^{(M)}$ and the ith inhomogeneity $\Omega^{(i)}$ is denoted as Γ_i. The matrix and the inhomogeneities are assumed to be individually homogeneous and have the linear thermal conduction behavior described by an isotropic Fourier's law:

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

Here, $\mathbf{q}^{(r)}$ and $\mathbf{e}^{(r)}$ represent the heat flux and intensity fields of phase $r\ (= M, 1, \ldots, m)$ and $k^{(r)}$ stands for the thermal conductivity of phase r. The intensity field $\mathbf{e}^{(r)}$ is related to the temperature field $\varphi^{(r)}$ by

$$\mathbf{e}^{(r)} = -\nabla\varphi^{(r)}. \tag{2}$$

In the absence of heat source, the heat flux vector $\mathbf{q}^{(r)}$ satisfies the following energy conservation equation

$$div\mathbf{q}^{(r)} = 0. \tag{3}$$

The interface between a generic inhomogeneity and the matrix is described by the general interface model initially proposed by Benveniste [15], Bövik [16] and then extended by Gu and He [17]. In order to specify the physical background of this interface model, we consider two configurations (Fig. 1). In the three-phase one (Fig. 1(a)), an inhomogeneity phase $\Omega^{(i)}$ is embedded in the matrix phase $\Omega^{(M)}$ via a thin interphase of uniform thickness h which is perfectly bonded to the matrix and inhomogeneity phases. In the two-phase one (Fig. 1(b)), the interphase is eliminated and replaced by a zero-thickness imperfect interface located at the middle surface Γ of the interphase and the matrix phase and the inhomogeneity phase are extended up to Γ so as to occupy the subdomains $\Omega^{(+)}$ and $\Omega^{(-)}$. The unit vector normal to Γ at $\mathbf{x} \in \Gamma$, noted as $\mathbf{n}(\mathbf{x})$, is oriented from the inhomogeneity phase to the matrix phase. By requiring that the temperature and normal flux jumps across the interphase in the three-phase one be, to within an error of order $0\left(h^2\right)$, equal to the corresponding jumps across the same zone in the two-phase one, and by applying the Taylor's expansion together with the continuous conditions of a perfect interface, the appropriate jumps across Γ are derived and characterized by the following relations [10,15]:

$$[\![\varphi]\!] = \varphi^{(+)} - \varphi^{(-)} = \frac{h}{2}\left[\left(\frac{1}{k^{(M)}} - \frac{1}{k^{(l)}}\right)q_n^{(+)} + \left(\frac{1}{k^{(i)}} - \frac{1}{k^{(l)}}\right)q_n^{(-)}\right], \tag{4}$$

$$[\![q_n]\!] = q_n^{(+)} - q_n^{(-)} = \frac{h}{2}\left[\left(k^{(l)} - k^{(M)}\right)\Delta_s\varphi^{(+)} + \left(k^{(l)} - k^{(i)}\right)\Delta_s\varphi^{(-)}\right]. \tag{5}$$

In these expressions, $[\![\bullet]\!]$ represents the interfacial jump operator defined by $[\![\bullet]\!] = \bullet^{(+)} - \bullet^{(-)}$ with $\bullet^{(+)}$ and $\bullet^{(-)}$ standing for the values of a quantity $\bullet$ evaluated at Γ on the inhomogeneity and matrix sides, respectively; q_n denotes the normal heat component given by $q_n = \mathbf{q}\cdot\mathbf{n}$; $k^{(i)}$, $k^{(M)}$ and $k^{(l)}$ stand for the thermal conductivities of the inhomogeneities, matrix and interphase.

Let $\langle\bullet\rangle$ be the interfacial average operator defined by $\langle\bullet\rangle = (\bullet^{(+)} - \bullet^{(-)})/2$. To simplify (4) and (5), recall the identities

$$(\bullet)^{(\pm)} = \langle\bullet\rangle \pm \frac{1}{2}[\![\bullet]\!]. \tag{6}$$

Applying (6) to (4) and (5), we obtain

$$[\![\varphi]\!] = \frac{h}{2}\left[\left(\frac{1}{k^{(M)}} - \frac{1}{k^{(l)}}\right)\left(\langle q_n\rangle - \frac{1}{2}[\![q_n]\!]\right) + \left(\frac{1}{k^{(i)}} - \frac{1}{k^{(l)}}\right)\left(\langle q_n\rangle + \frac{1}{2}[\![q_n]\!]\right)\right], \tag{7}$$

$$[\![q_n]\!] = \frac{h}{2}\left[\left(k^{(l)} - k^{(M)}\right)\Delta_s\left(\langle\varphi\rangle - \frac{1}{2}[\![\varphi]\!]\right) + (k^{(l)} - k^{(i)})\Delta_s\left(\langle\varphi\rangle + \frac{1}{2}[\![\varphi]\!]\right)\right]. \tag{8}$$

Taking into account the fact that the jump $[\![\bullet]\!]$ of any quantity $(\bullet)$ involved in the right-side members of these two equations is of

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