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Effective conductivity of spheroidal particle composite with imperfect interfaces: Complete solutions for periodic and random micro structures

V.I. Kushch [a,*], Igor Sevostianov [b], A.S. Belyaev [a]

[a] Institute for Superhard Materials of the National Academy of Sciences, 04074 Kiev, Ukraine
[b] Department of Mechanical Engineering, New Mexico State University, PO Box 30001, Las Cruces, NM 88003, USA

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ABSTRACT

The rigorous analytical approach to the conductivity homogenization problem for spheroidal particle composite with imperfect interfaces has been developed. The complete multipole series solution for a single inclusion with imperfect interface constitutes mathematical background of the work and provides a basic building block for the Maxwell and Rayleigh homogenization schemes. The low- and highly conducting spheroidal interface are considered in a unified way. The developed theory enables an analysis of composites of periodic and random micro structure with imperfect interfaces. Numerical study shows quite a significant combined effect of micro structure and imperfect interfaces on the macroscopic conductivity of composite. The obtained accurate solution serves as a benchmark for the known approximate theories. Their error due to neglecting the interaction effects and simplified treating the imperfect interfaces is estimated.

1. Introduction

The typical structure parameters entering formulas for the effective properties of heterogeneous solids are the phase properties, volume content and shape of inhomogeneities. This list is not complete, of course. Two other, less often considered though in no way less important, factors are the micro structure (arrangement of inclusions) and matrix-to-inclusion interface bonding type. First, the effective properties of composite are generally structure-dependent. This effect is entirely due to interactions between the inclusions, so taking them into account is a prerequisite for accurate predicting the composite's behavior. Second, the adopted commonly "perfect interface" idealization rarely occurs in practice. The real interface is always imperfect due to the atomic lattices mismatch, phonons scattering, poor mechanical or chemical adherence, surface contamination, oxide and interphase diffusion/reaction layers, debonding, etc. These phenomena affect the effective properties of composite and make them size-dependent and so must be taken into account in the predictive model.

In the heat conduction problem we consider, an imperfect thermal contact between the inclusions and surrounding matrix is typically described by the low-conductive (LC) interface model. Known also as the Kapitza resistance, it assumes the normal heat flux be continuous through the interface whereas the temperature jump is non-zero and proportional to the normal flux (e.g., Hasselman and Johnson, 1987). On the contrary, the high-conductive (HC) interface model (Torquato and Rintoul, 1995) assumes continuity of temperature and jump of normal heat flux, taken to be proportional to the surface temperature (Cheng and Torquato, 1997) or surface Laplacian of

* Corresponding author.
E-mail addresses: vkushch@bigmir.net (V.I. Kushch), igor@nmsu.edu (I. Sevostianov).

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temperature (Lipton, 1997, 1998; Miloh and Benveniste, 1999, among others). Noteworthy, both LC and HC model of imperfect interface can be derived as limiting cases of a thin interphase layer (e.g., Miloh and Benveniste, 1999). The dual interface model (Pavanello et al., 2012) implements more complex interface behavior, observed in recent investigations on nanocomposites (e.g., Minnich and Chen, 2007; Ordonez-Miranda et al., 2011).

Mathematical complexity of these problems is due to the fact that the interface conditions involve the local curvature of interface. Not surprisingly, most of the work is done on the composites with imperfect interfaces of constant curvature (spherical and circular). Hasselman and Johnson (1987) have extended Maxwell's formula for the effective conductivity to the composites with LC imperfect interface. The same formula has been derived using the self-consistent scheme and Mori–Tanaka approach (Benveniste, 1987). The second order, $O(c^2)$ correction to these results requires taking the pair interactions into account (Chiew and Glandt, 1987). An effect of interface parameters on the overall thermal conductivity of periodic composites has been studied accurately by Rayleigh's method for LC (Torquato and Cheng, 1997) and HC (Cheng and Torquato, 1997) cases. The rigorous bounds on the effective thermal conductivity of random composite have been given (Torquato and Rintoul, 1995) in terms of the phase contrast between the inclusions and matrix, the interface strength and higher-order morphological information. We mention also the reciprocal relations linking the effective conductivity of composite with HC interfaces to that of a composite with the same phase geometry but with LC interfaces (Lipton, 1997a).

The composites with non-spherical imperfect interfaces have been much less explored. The first order approximations for the effective thermal conductivity of composite with arbitrarily oriented ellipsoidal inclusions were obtained using the Mori–Tanaka (Dunn and Taya, 1993; Nan et al., 1997) and Maxwell (Duan and Karihaloo, 2007) averaging schemes. In these and other similar works, an effect of imperfect interface is taken into account approximately, by replacing an imperfect interface with a thin coating of variable thickness defined by two confocal spheroids. The papers by Benveniste and Miloh (1986) and Miloh and Benveniste (1999) are probably the only works where the imperfect ellipsoidal interfaces were properly taken into account. There, the formulas for effective conductivity of composite with low- (Benveniste and Miloh, 1986) and highly conducting (Miloh and Benveniste, 1999) interfaces at low concentration limit have been derived. Some approximate results for finite concentrations have been also obtained (Miloh and Benveniste, 1999).

Another common drawback of the mentioned "single inclusion" models of composite is their insensitivity to microstructure whereas an effect of particle interactions is taken via approximate schemes. Their applicability is hence limited to composites with low volume content of disperse phase. In the present paper, the multipole expansion approach has been applied to obtain a complete solution to the homogenization problem for a spheroidal particle composite with imperfect interface. The developed theory provides an accurate estimate of the effective conductivity of composites with periodic and random arrangements of spheroidal inclusions, with low- and highly conducting interfaces.

2. Problem statement

We consider the thermal conductivity homogenization problem for the matrix type composite consisting of a homogeneous solid (matrix) containing identical, equally oriented spheroidal inclusions. Both the matrix and the inclusions are isotropic. The governing equation is $\nabla \cdot \mathbf{q} = 0$, where $\mathbf{q} = -k\nabla T$ is the heat flux vector, k is the thermal conductivity, T and ∇T are the temperature and its gradient. In the case of constant k, T obeys Laplace equation $\nabla^2 T = 0$. All the matrix- and inhomogeneity-related quantities are indexed by "0" and "1", respectively: $T = T^{(0)}$ and $k = k_0$ in the matrix, $T = T^{(1)}$ and $k = k_1$ in the inhomogeneities. The thermal load is defined by the far/mean temperature gradient $\mathbf{G} = G_j \mathbf{i}_j$ where $\mathbf{i}_j$ are the unit vectors of the Cartesian coordinate system. The corresponding far/averaged temperature field is $T_{far} = \mathbf{G} \cdot \mathbf{x}$.

Two kinds of imperfect thermal contact between the matrix and inclusions are considered. The low-conducting (LC) interface assumes continuity of the normal heat flux and jump of temperature across the interface. The relevant boundary conditions are

$$h_c[[T]]_S + q_n = 0; \quad [[q_n]]_S = 0; \tag{1}$$

where $q_n = -k\nabla T \cdot \mathbf{n} = -k\frac{\partial T}{\partial n}$ is the normal flux and $[[T]]_S = \left(T^{(0)} - T^{(1)}\right)|_S$ means a jump of temperature T across the interface S. The coefficient h_c with dimensionality $[\mathrm{Wt}/(\mathrm{m}^2\mathrm{K})]$ is known as the surface conductivity. An opposite case is the highly conducting (HC) interface where temperature is continuous across the interface whereas normal heat flux jump is proportional to the surface Laplacian of temperature $\Delta_s T = \mathbf{n} \cdot \nabla \times (\mathbf{n} \times \nabla T)$:

$$[[T]]_S = 0; \quad [[q_n]]_S - h_s \Delta_s T^{(1)} = 0. \tag{2}$$

Here, $[[q_n]]_S = \left(q_n^{(0)} - q_n^{(1)}\right)|_S$ and h_s is the coefficient with dimensionality $[\mathrm{Wt}/\mathrm{K}]$. For derivation and discussion on the physical nature of (2), see Miloh and Benveniste (1999). Here, we mention only that the dimensionality analysis (e.g., Benveniste and Miloh, 1986) predicts dependence of the composite behavior on the size of inhomogeneities in both LC and HC cases. This "size effect" vanish only for the extreme values $h_c = \infty$ in (1) and $h_s = 0$ in (2) where they reduce to the conventional, perfect interface bonding condition.

Our task is to evaluate the effective conductivity tensor $\mathbf{K}^* = k^*_{ij}\mathbf{i}_i\mathbf{i}_j$ of the spheroidal particle composite with imperfect interface.