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Interacting ellipsoidal inhomogeneities by multipole expansion method and effective conductivity of particulate composite

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ABSTRACT

The complete series solution has been obtained for the potential field of an array of ellipsoidal inhomogeneities regarded as a multi particle model of composite. By combining the superposition principle, the perturbation field expansion in terms of ellipsoidal harmonics and the re-expansion formulas for them, the model boundary value problem is reduced to a set of linear algebraic equations. The obtained solution has been implemented in the modified Maxwell and Ralyeigh homogenization schemes for effective conductivity of ellipsoidal particle composite with an adequate account for the interaction effects. The results of numerical study are provided which illustrate the convergence rate of solution and accuracy of the developed method.

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1. Introduction

An ellipsoid is probably the most popular in the micromechanics model shape of inhomogeneity for it provides considering, within the unified formalism, a wide range of heterogeneous solids including porous and composite media with round/spherical inhomogeneities, short fibers, platelets, elliptical cracks, etc. The Eshelby's solution (Eshelby, 1959) for a single ellipsoidal inclusion in an infinite medium constitutes the theoretical background of many micromechanical theories and hitherto is widely used. The Eshelby model based theories provide a satisfactory prediction of the effective properties of composites with low-to-moderate volume content of inhomogeneities where interactions between the inhomogeneities can be safely neglected. On the contrary, behavior of high-filled composite is determined, to a large extent, by interaction of adjacent inhomogeneities producing high gradients of local fields and affecting quite significantly the effective properties. The predictive models for these composites, in order to account for the interaction of inhomogeneities, should employ the multi particle structure models and rigorous methods of their analysis.

Several multi particle models of composites with inhomogeneities of spherical and spheroidal shape are available in literature. We mention only a few papers where the two-particle (Chiew & Glandt, 1987; Jeffrey, 1973; Lu & Kim, 1990) and periodic (Cheng & Torquato, 1997; Kushch, 1997; McPhedran & McKenzie, 1978; Rayleigh, 1892; Sangani & Acrivos, 1983) models of particulate composite were studied. At the same time, interaction of ellipsoidal inhomogeneities as well as its effect on the effective properties of composite is hitherto hardly studied.

The paper by Moskovidis and Mura (1975) is probably the first one where an interation of two ellipsoidal inhomogeneities was addressed. An approximate solution obtained there is based on the equivalent inclusion method

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(Eshelby, 1959) and hence is valid only for far-separated inhomogeneities. A few subsequent publications in this direction, they are Chen and Yang (1995) in conductivity and Kirilyuk (2001), Shodja, Rad, and Soheilifard (2003) and Bedayat and Taleghani (2015) in elasticity context, do not show any significant progress in comparison with Moskovidis and Mura (1975). To the best author's knowledge, all the available homogenization schemes for composites with ellipsoidal inhomogeneities employ the single-particle structure model. In the conductivity context, they are Fricke (1924), Benveniste and Miloh (1986), Miloh and Benveniste (1999) and Shafiro and Kachanov (2000), to mention a few.

In the present work, a complete full field solution for an unbounded solid containing an array of ellipsoidal inhomogeneities has been obtained by the Multipole Expansion Method (Kushch, 2013). By combining (a) superposition principle, (b) multipole expansion of perturbation fields of inhomogeneities in terms of ellipsoidal harmonics and (c) translation type re-expansion formulas for these harmonics, the boundary value problem for heterogeneous solid is reduced to an infinite algebraic system with respect to the multipole moments of ellipsoidal inhomogeneities. The obtained solutions for a finite cluster and an infinite periodic array of inhomogeneities are implemented in two classical homogenization schemes originated by Maxwell (1873) and Rayleigh (1892).

2. Potential field of interacting ellipsoids

2.1. Problem statement

We consider the conductivity problem for an unbounded solid, or matrix, containing a certain number of ellipsoidal inhomogeneities and regarded as a multi particle, or cluster, model of particulate composite. Here, the term "conductivity" applies to all transfer (heat, charge, mass, etc.) phenomena whose potential obeys Laplace equation. To be specific, we use terminology of the thermal conductivity theory. Both the matrix and inhomogeneities are made of isotropic materials. 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, $\nabla^2 T = 0$.

To keep our presentation clear, we minimize the number of the model parameters. To this end, we assume that all the inhomogeneities are of the same shape, size, properties and orientation. 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 base vectors of the Cartesian coordinate system. The corresponding far/mean temperature field is $T_{far} = \mathbf{G} \cdot \mathbf{x}$.

The perfect thermal contact between the matrix and inhomogeneities is assumed which means the temperature and normal heat flux continuity at the interface *S*. The relevant boundary conditions are

$$[[T]]_{S} = 0; \quad [[q_{n}]]_{S} = 0; \tag{1}$$

where $q_n = -k\nabla T \cdot \mathbf{n} = -k\frac{\partial T}{\partial n}$ is the normal flux and $[[f]]_S$ is a jump of quantity f across the interface S with outer normal vector \mathbf{n} . Our aim is to obtain the accurate full field solution to the boundary value problem and apply it for evaluation of the effective conductivity tensor $\mathbf{K}^* = k_{ij}^* \mathbf{i}_i \mathbf{i}_j$ of the ellipsoidal particle composite.

2.2. Single ellipsoidal inhomogeneity

Consider first an unbounded domain containing a single ellipsoidal inhomogeneity with the semiaxes $a_1 > a_2 > a_3$ oriented along the corresponding axes of Cartesian coordinate system $Ox_1x_2x_3$. For the ellipsoidal coordinates and other notations, see Appendix A. Noteworthy, in the ellipsoid-related notations we follow the recent monograph by Dassios (2012). The temperature field in and outside the inhomogeneity is caused by the far temperature field T_{far} : $T^{(0)} \rightarrow T_{far}$ when $\|\mathbf{r}\| \rightarrow \infty$. To complete the problem formulation, we require that $T^{(1)}(0) = 0$. We are looking for the temperature fields inside and outside the inhomogeneity.

The regular temperature field inside the inhomogeneity is given by a series of interior solid harmonics \mathbb{E}_n^m defined by Eq. (A.1) of Appendix A:

$$T^{(1)}(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=1}^{2n+1} D_{nm} \mathbb{E}_n^m(\mathbf{r}).$$
(2)

Here, D_{nm} are the inhomogeneity-related series expansion coefficients. The temperature field outside the inhomogeneity is written as a sum of the far field T_{far} and perturbation field $T_{per}(\rightarrow 0 \text{ for } ||\mathbf{r}|| \rightarrow \infty)$ caused by the inhomogeneity. The series expansion of T_{far} is analogous to Eq. (2) and involves only the interior harmonics \mathbb{E}_1^m :

$$T_{far} = \mathbf{G} \cdot \mathbf{r} = \sum_{m=1}^{3} G_m \frac{h_m}{h_1 h_2 h_3} \mathbb{E}_1^m(\mathbf{r}) = \sum_{m=1}^{3} \widetilde{G}_m \mathbb{E}_1^m(\mathbf{r}),$$
(3)

where $\widetilde{G}_m = G_m/H_m$ and $H_m = (h_1h_2h_3)/h_m$.

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