International Journal of Engineering Science 74 (2014) 15–34

Contents lists available at ScienceDirect

International Journal of Engineering Science

journal homepage: www.elsevier.com/locate/ijengsci

Dipole moments, property contribution tensors and effective conductivity of anisotropic particulate composites

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ARTICLE INFO

Article history:
Received 4 June 2013
Received in revised form 22 July 2013
Accepted 7 August 2013
Available online 23 September 2013

Keywords:
Homogenization problem
Anisotropy
Dipole moment
Contribution tensor
Effective conductivity

ABSTRACT

The paper addresses the homogenization problem for a particulate composite with anisotropic constituents. Its specific goal is to bridge the gap between two different approaches to the problem of homogenization focusing on the anisotropic materials and to identify and discuss the key microstructural parameters affecting overall conductivity of heterogeneous materials. The basic concepts of the homogenization theory including a consistent way of introducing the macroscopic field parameters are discussed and clarified. The exact explicit relations have been obtained between the dipole moments, property contribution tensors and effective conductivity of composite with phase anisotropy of the general type. A detailed comparison of the analytical expressions for the dipole moments obtained by the multipole expansion method and the independently derived expressions for the conductivity contribution tensors has been made between and their equivalence is shown for the matrix type composites with transversely isotropic constituents and spheroidal inhomogeneities. The numerical examples illustrate effect on the overall conductivity of particulate composite of the properties of constituents, shape, volume content, spatial arrangement and orientation of particles.

1. Introduction

The homogenization problem of the theory of conductivity[1] is probably the oldest and best explored area in the science of heterogeneous media. This long history traces back to 19th century and to the pioneering works by Poisson, Faraday, Maxwell, Mossotti, Clausius and Lorenz, see review of Markov (2000). Since that time, several approaches have been developed to evaluate effective transport properties of heterogeneous solids and fluids. Various aspects of the problem were discussed in many books and papers; however, this work is still far from completion.

The macroscopic, or effective, conductivity tensor $\mathbf{K}^* = k^*_{ij}\mathbf{i}_i \otimes \mathbf{i}_j$ is defined by Fourier law for macro level:

$$\langle \mathbf{q} \rangle = -\mathbf{K}^* \cdot \langle \nabla T \rangle. \tag{1.1}$$

where $\langle \nabla T \rangle$ and $\langle \mathbf{q} \rangle$ are the macroscopic temperature gradient and heat flux vector, respectively. Evaluation of $\mathbf{K}^*$ commonly uses the formula (Batchelor, 1974)

$$\langle \mathbf{q} \rangle = -\mathbf{K}_0 \cdot \langle \nabla T \rangle + n\langle \mathbf{p} \rangle, \tag{1.2}$$

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[1] Hereafter, conductivity is understood in a broad sense covering the "transport" type physical (thermal, dielectric, optical, etc.) phenomena. To be specific, we will use terminology of the heat conduction theory.

0020-7225/$ - see front matter
http://dx.doi.org/10.1016/j.ijengsci.2013.08.002

where $\mathbf{K}_0$ is the conductivity tensor of matrix material, n is a number density (average number of particles per unit volume) and $\mathbf{p}$ is defined by Batchelor as "*a measure of the net additional dipole strength ... resulting from the replacement of matrix material there by particle material*". Specifically,

$$\mathbf{p}_i = \int_{V_i} (\mathbf{q} - \mathbf{q}_0) d\mathbf{x} = (\mathbf{K}_0 - \mathbf{K}_1) \cdot \int_{V_i} \nabla T d\mathbf{x}, \tag{1.3}$$

where V_i and A_i is the volume and surface area, respectively, of ith inhomogeneity with conductivity $\mathbf{K}_1$ and $\mathbf{q}_0 = -\mathbf{K}_0 \cdot \nabla T$ (Batchelor, 1974). The value of the induced dipole moment $\mathbf{p}$ depends on the size, shape, orientation and properties of this particle as well as all other particles in the mixture. Due to linearity of the considered problem, $\mathbf{p}_i = -\mathbf{H}_i \cdot \langle \nabla T \rangle$, where $\mathbf{H}_i$ is the particle-related second rank tensor. From Eqs. (1.1) and (1.2) one readily obtains $\mathbf{K}^* = \mathbf{K}_0 + n\langle \mathbf{H}_i \rangle$ and thus determination of the effective transport properties of composite reduces to the determination of the mean particle parameter, $\mathbf{p}$ or $\mathbf{H}$.

Alternative approach consists in using one-particle solution (Fricke, 1924) and accounting for interaction between particles through placing a single inhomogeneity into certain "effective environment" – either effective media or effective field (Markov, 2000). Note, that both approaches – multipolar expansion and single particle approximations – use the same idea: representation of the effect of inhomogeneity in terms of the generated far field. For elastic case, it was shown by Sevostianov and Kachanov (2011). This connection is not always well understood that produces at least two lines of research rarely interacting with each other. It leads, in turn, to repetitions of the results formulated in different terminologies.

Presently, most of the results on conductivity of heterogeneous media are related to macroscopically isotropic materials. At the same time, anisotropy is commonly observed in natural and man-made materials and thus should be taken into account properly. Macroscopic anisotropy origin is due to (a) shape and orientation of inhomogeneities (e.g., Shafiro & Kachanov, 2000; Kushch & Sangani, 2000); (b) their arrangement (e.g., Sen & Torquato, 1989) and (c) anisotropy of phase materials.

A few publications are available on conductivity of composites with anisotropic constituents. Willis (1977) has derived the Hashin–Shtrikman type bounds and self-consistent estimates for the overall properties of composites with statistical homogeneous and isotropic microstructure and anisotropic phases. The Maxwell type homogenization approach has been used by Sihvola (1997) to evaluate an effective dielectric permittivity of spherical particle composite with anisotropic constituents. An effective thermal conductivity of transversely isotropic media with arbitrary oriented ellipsoidal inhomogeneities was studied by Giraud, Gruescu, Do, Homand, and Kondo (2007) who combined the Mori–Tanaka scheme with numerical integration procedure for the Hill's tensor. An asymptotic formula for the effective property of the dilute anisotropic composite has been derived (Ammari, Kang, & Kim, 2005) based on the layer potential technique and 2D unit cell model. Helsing and Samuelsson (1995) have applied the Fredholm integral equation method to get an accurate numerical solution of the two dimensional conductivity problem for a periodic composite of arbitrarily shaped anisotropic inhomogeneities in an anisotropic matrix. The multipole expansion method has been applied by Kushch (1997) to study local fields and effective conductivity of a periodic aligned spheroidal particles composite with the transversely isotropic constituents. In the latter work, all three anisotropy sources – phase properties, shape of particles and their arrangement – have been taken into account.

The goal of the present paper is to bridge the gap between two different approaches – multipolar expansion and single particle approximations – to the problem of homogenization focusing on the anisotropic materials and to identify and discuss the key microstructural parameters controlling the overall conductivity of heterogeneous materials.

2. Background results

The governing equations of local steady-state transport (heat conduction, to be specific) in the composite are

$$\nabla \cdot \mathbf{q}^{(i)} = 0, \quad \mathbf{q}^{(i)} = -\mathbf{K}_i \cdot \nabla T^{(i)}. \tag{2.1}$$

Here, $T^{(i)}$ is the temperature, $\mathbf{q}^{(i)}$ is the heat flux and $\mathbf{K}_i$ is the conductivity tensor of ith phase ($i = 0$ for matrix, $i = 1$ for inhomogeneities). Both the matrix and inhomogeneities are anisotropic. For simplicity sake, our study is restricted to two-phase composites: generalization to the multiple phase composite is straightforward. We consider macroscopically uniform temperature field in a composite that implies constancy of the corresponding macroscopic gradient $\langle \nabla T \rangle$ and heat flux $\langle \mathbf{q} \rangle$ vectors. This problem statement provides determining the macroscopic, or effective, conductivity tensor. This is well-known – but still not always correctly formulated - problem. Therefore, some basic concepts of the homogenization theory including a consistent way of introducing the macroscopic field parameters are clarified first.

2.1. Definition of macroscopic quantities: volume vs. surface averaging

The macroscopic quantities $\langle \nabla T \rangle$ and $\langle \mathbf{q} \rangle$ are commonly taken as the volume-averaged values of the corresponding local fields:

$$\langle \nabla T \rangle \overset{def}{=} \frac{1}{V} \int_V \nabla T d\mathbf{x}; \quad \langle \mathbf{q} \rangle \overset{def}{=} \frac{1}{V} \int_V \mathbf{q} d\mathbf{x}; \tag{2.2}$$