



On the effect of inclusion shape on effective thermal conductivity of heterogeneous materials



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ABSTRACT

In this paper, a numerical homogenization technique is used to estimate the effective thermal conductivity of random two-dimensional two-phase heterogeneous materials. The thermal computational leads essentially bring out the effect of the voids/inclusions morphology on the effective physical properties. This is achieved using two different heterogeneous materials: microstructure 1 with non-overlapping spherical pores and microstructure 2 with non overlapping spherical rigid inclusions taking into account five different volume fractions from each case. The notion of the representative volume element is introduced for numerical simulations using periodic boundary conditions and uniform gradient of temperature conditions. The obtained effective material properties on the representative microstructures are compared with different analytical models as: series model, parallel model, effective medium theory and Maxwell models, for different morphologies of rigid inclusions and voids. This paper compares the performance of several classical effective medium approximations. Finally, an analytical expression developing the Maxwell model is proposed to estimate the effective thermal conductivity of heterogeneous materials taking into account the inclusion morphology.

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1. Introduction

The Effective Thermal Conductivity (ETC) of two-phase materials (matrix and inclusions) is one of the most important quantities characterizing energy transport in a vast range of industrial and engineering applications. Lots of investigations have been on the estimation of the ETC of two-phase materials, Whitaker (1999) and Wang and Pan (2008). These present methods are divided into the analytical models and the numerical simulations, Coquard and Baillis (2009). The analytical models of Maxwell (1873) and Othuman and Wang (2011), were generally based on a geometrical

simplification of the microstructure and assumed regular arrangements of the solid phase and the air phase, rather than random mixtures. The numerical models were based on mathematical computation of the microstructure describing the material phases, Veisoh et al. (2009). Another common way of estimating effective thermal conductivity for heterogeneous materials with known microstructures is to make rigorous numerical simulations using the finite difference method, the finite element method, or other numerical techniques, Divo et al. (2000), Rocha and Cruz (2001) and Bolot et al. (2005).

For the analytical models, the early work of Maxwell (1873) proposed a model for low dispersion of particles but neglecting particle–particle interactions and can only be applied to structures with dilute particle dispersion. Several attempts have been made to develop expressions for effective thermal conductivity of two-phase materials by various

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researchers such as: Rayleigh (1892), Wiener (1904), Lewis and Nielsen (1970), Cunningham and Peddicord (1981), Torquato (1985), Hadley (1986), Agari and Uno (1986), Misra et al. (1994) and Singh and Kasana (2004). Rayleigh (1892) pioneered a new formalism that furnishes an analytical solution for a periodic array of spherical and cylindrical inclusions in a uniform matrix. This has proven a major improvement to Maxwell's theory in predicting the ETC over a large range of particle volume fractions up to close packing, McPhedran and McKenzie (1978) and McKenzie et al. (1978). Rayleigh's idea has been studied extensively by many authors for decades. Wiener equations gave the maximum and minimum value by parallel and series models. McKenzie et al. (1978) extended Rayleigh's method accounting for arbitrarily high order multi-poles to calculate the thermal conductivity of simple body-centered and face-centered cubic lattices of conductive spheres distributed in a matrix. Zimmerman (1996) derived an analytical expression for the ETC of a two-dimensional medium with randomly distributed and randomly oriented elliptical inclusions using equivalent inclusion based methods. Cheng and Torquato (1997) further generalized Rayleigh's method by considering imperfect interfaces. Lewis and Nielsen (1970) reported a semi-empirical model incorporating the effect of the shape and the orientation of particles. Other approach for thermal conductivity predictions was initiated by Torquato (1985) for dispersed spherical and cylindrical particles. This approach also takes into account the filler geometry and the statistical perturbation around each filler particle. Agari and Uno (1986) have proposed another semi-empirical model which is based on the argument that the enhanced thermal conductivity of highly filled composites originates from forming conductive chains of fillers. The self-consistent scheme (SCS) is another method with general applicability. It considers a heterogeneous medium as being composed of a basic element embedded in an equivalent homogeneous medium, with an effective conductivity whose value is determined through a linear relationship between the effective heat flux and temperature gradient effect in a similar manner to a homogeneous material, Hashin (1968).

More recently, many works started to focus on the evaluation of the effective thermal conductivity, given its importance. For example, Yang et al. (2013) developed a generalized self consistent model to predict the effective thermal conductivity of composites reinforced with multi-layered orthotropic fibers. A new analytical solution to predict the ETC is developed by Akbari et al. (2013) for anisotropic materials based on the self consistent field concept. Florez et al. (2013) proposed a model to estimate the effective thermal conductivity of sintered porous media for heat pipes. The electrical circuit analogy is employed to determine the heat leaving the top and reaching the bottom of the cell. A new effective medium theory was proposed to model the thermal conductivity of porous materials by Gong et al. (2014) using a simple algebraic expression for thermal conductivity which can unifies the five basic structural models : parallel, series, two forms of Maxwell's and the effective medium theory.

Nowadays, and with the development of technology, great attention is paid to porous/composite materials for their widespread industrial applications. Many numerical models

have been used for predicting their ETC, see Verma et al. (1991), Veyret et al. (1993), Pabst and Gregorova (2006) and Coquard and Baillis (2009). For example, Verma et al. (1991) developed a porosity dependence correction term for spherical and non-spherical particles. Veyret et al. (1993) used a numerical approach to determine the ETC of the diphasic medium. Calmidi and Mahajan (1999) presented a one-dimensional heat conduction model, considering the porous medium to be formed of two-dimensional array of hexagonal cells. Rocha and Cruz (2001) calculated ETC of unidirectional fibrous composite materials with an interfacial thermal resistance between the continuous and dispersed components. Bhattacharya et al. (2002) extended the analysis of Calmidi and Mahajan, for metal foams of a complex array of interconnected fibers with an irregular lump of metal at the intersection of two fibers. Pabst and Gregorova (2006) developed a simple second-order expression for the porosity dependence of thermal conductivity. Wang and Pan (2008) developed a random generation-growth method to reproduce the microstructures of open-cell foam materials via computer modeling and so on.

Most of the heat transfer works in the literature treats equally all composites materials and porous media, independently of their inclusion morphology. The main purpose of this work is to bring out the influence of the inclusion morphology on the effective thermal conductivity. The finite element method (FEM) is used to evaluate the effective thermal conductivity of random 2D, two phase heterogeneous materials. The first microstructure is a porous medium, and the second is a non porous composite materials. The computational results are compared with different analytical models. The comparison clearly shows that the effect of the inclusions morphology on thermal conductivity is observed only for porous medium, where the Maxwell's model does not provide an acceptable estimate except for circular voids. In the case of composite materials, the Maxwell's model is still valid gives a very good estimation independently of the inclusions morphology. Finally, an analytical formula taking into account the inclusion morphology is proposed, to estimate the effective thermal conductivity of heterogeneous materials.

2. Computational thermal homogenization

In this section, all elements and notations of numerical homogenization necessary to determine the effective thermal conductivity, using the methodology explained by Kanit et al. (2003) based on the FEM, are carried out.

2.1. Microstructures generating and thermal conductivity of phases

The morphology and technique of 2D microstructures generating is presented in this section. For each studied microstructure, five configurations with different populations of inclusion shapes are investigated. Each microstructure contains one population of non-overlapped inclusions, randomly distributed and randomly oriented in a continuous matrix. It should be noted that there is no contact between neighboring inclusions of the dispersed phase. The notations used are $P_1 = P$ and $P_2 = 1 - P$ for the volume (surface in 2D)

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