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Effective thermal conductivity of functionally graded random micro-heterogeneous materials using representative volume element and BEM

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ABSTRACT

This work introduces a numerical methodology for the computation of the effective thermal conductivity (ETC) of random micro-heterogeneous materials using representative volume elements and the Fast Multipole Boundary Element Method (FMBEM). The methodology is applied to solve two-dimensional foam-like materials consisting of random distributions of circular isolated holes. The computed ETC values are successfully used to predict the temperature fields of two materials with functionally graded ETCs. Numerical and analytical results are experimentally validated. The proposed methodology is flexible and versatile, as it is capable to account for both, the geometrical and topological details of the material microstructure.

1. Introduction

Effective thermal conductivity (ETC) of micro-heterogeneous materials has been an active research field for over a century. The importance of micro-heterogeneous materials like granular metals and ceramics [1], fibrous composites [2], or polymeric open-cell foams [3] lies in their applications in high performance insulations [4,5], packed beds, heterogeneous catalysts [6], composite materials and powder metallurgy [7]. The size, shape, physical properties and spatial distribution of the micro-structural constituents largely determine the macroscopic, overall behavior of these multi-phase materials. From the point of view of materials design, it would be highly attractive to tailor the material microstructure in order to obtain the desired set of macroscopic properties. One remarkable example of this concept can be found in the so-called functionally graded materials (FGM), where particular spatial variations of local material properties can be used to generate materials with a set of unique properties. The local composition of the microstructure in a composite material can be varied to obtain certain change in the local material property. For example, thin layer FGM electric/thermal ceramic systems are almost a commercial reality today [4]. The FGM concept could also be used in the production of thermoplastic polymeric foams for thermal insulation. Foams can be assimilated to a micro-heterogeneous material consisting of a thermoplastic polymer matrix that contains small cells filled with gas that may constitute an important fraction of the total volume [8]. The spatial distribution of the gas cells modifies the heat conduction properties along the material.

Several models for the computation of the ETC of micro-heterogeneous materials have been proposed in the literature. A recent review on this subject is due to Wang and Pan [9] who made a comprehensive and critical review of the most important existing models. The authors classified those models in two main groups, *theoretical* and *numerical*, the former are further subdivided in two-phase and multiphase models. The two-phase models are of interest for this work. Following Wang and Pan, two-phase models are classified into *basic*, *combined* and *network models*. The *basic models* are based on physical principles which have a closed form solution (either exact or approximate). Some examples are the Parallel, Series, the two forms of the Maxwell–Eucken model and the Effective Medium Theory (EMT) [10]. These models are theoretically based and they depend only on the volume fraction and thermal conductivity of the micro-structural constituents; on the other hand they represent idealized microstructures that can only be found in very specific cases [10–13]. Series and Parallel models assume that the physical arrangement of the components is either perpendicular or parallel to the heat flux. Alternatively, the Maxwell–Eucken model assumes a two-component dilute dispersion of spherical particles, that is, the distance between the particles is large enough to avoid distorting the local temperature field of each other (non-interacting). Overall, the Maxwell–Eucken model is unable to make predictions for high concentrations of particles where the local temperature distortions affect those of the neighboring inclusions. Two forms of the Maxwell–Eucken (M–E) model arise depending on the relative values of thermal conductivity of the continuous and the dispersed phases. The M–E 1 form is

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Nomenclature

A	area (mm^2)
Bi	Biot number
C	characteristic length (m)
e	emittance
f	void fraction
h	heat transfer coefficient ($W\,m^{-2}\,C^{-1}$)
k	thermal conductivity ($W\,m^{-1}\,C^{-1}$)
K	effective thermal conductivity ($W\,m^{-1}\,C^{-1}$)
L	side length (mm)
m	number of discrete f values in the FGM models
n	number of zones in the FGM models
N	number of degrees of freedom of the FMBEM model
Q	heat flux ($W\,m^{-2}$)
r	hole radius (mm)
T	temperature (°C)
x	x-coordinate (mm)
y	y-coordinate (mm)

Greek symbols

α	K/k_0 effective thermal conductivity relative to the matrix material

Subscripts

0	matrix material
1, 2	boundary condition identifier
disp	dispersed phase
envr	environment
i	discrete value identifier
r	radiation transfer
surf	surface

adopted if the conductivity of the matrix, k_0, is greater than the conductivity of the dispersed phase, k_{disp}, and the M–E 2 form comes up if $k_0 < k_{disp}$. Conversely, the EMT model assumes a completely random distribution of the components, with neither phase being continuous or dispersed. Besides, the effect of local distortions to the temperature distribution is averaged such that the temperature over the material is uniform. In this way, the conductivity assigned is an effective value. *Combined models* consist of the weighted mean of basic models using empirical parameters [8,10,14,15]. Thus, if experimental data is available these models provide accurate results, but they are actually non-predictive. Such models require extensive experimental data to estimate parameters that may have no physical significance. Finally, the *network models* are similar to the *combined models* in the sense they combine *basic models*, but they use much more complex arrangements connecting series or parallel elements to render the microstructure of a heterogeneous material. They are only employed for certain complex materials, such as soil or filled polymers [9].

The limitations of the above-mentioned models have driven efforts toward computational approaches (*numerical methods* in Wang and Pan classification [9]) that progressively incorporate physically-meaningful higher-level description of the micro-scale. The work load is then shifted to high performance computational methods such as BEM [16], FEM [17] and Lattice Boltzmann [18]. The structural details of every phase, as shape and size distributions, can be described in detail, and only the thermal conductivity of the phases must be determined separately. Thus, heterogeneous materials with any structural topology and thermal properties can be simulated.

The computational modeling of the material microstructure together with homogenization techniques are widely used to predict the macroscopic behavior of heterogeneous materials [17,19]. Most of the homogenization approaches make an assumption on global periodicity of the microstructure details, suggesting that the whole macroscopic specimen consists of spatially repeated unit cells [19]. A somewhat more realistic approach for the homogenization of randomly distributed phases, is to use statistically representative volume elements (RVE). In order to make the computed results reliable, the RVE sample must be selected small enough to be considered as a material point with respect to the size of the domain under analysis, but large enough to be a statistically representative sample of the microstructure. Thus, a RVE usually contains a large number of heterogeneities, and therefore the computations could be expensive. However, the computational effort is small when compared to that of the direct calculation for the complete problem domain [17].

The aim of this work is to develop a numerical approach for the prediction of the thermal conductivity of functionally graded micro-heterogeneous materials. To this end, a methodology based on the numerical modeling of RVE using the Boundary Element Method (BEM) is introduced. The Boundary Element Method (BEM) is widely used to solve many engineering problems due to its simplicity in the mesh generation, restricted only to the boundaries, and accuracy as it calculates the derivative of the potential in exact form [16]. To further improve the performance of the BEM, the Fast Multipole Boundary Element Method is used in this work to reduce the computational cost in terms of both, operations and memory requirements with respect to direct BEM formulations [21].

With the purpose of testing the predictive capabilities of the proposed methodology, two foam-like functionally graded materials are analyzed. The FGM consist of circular holes distributed in a high-thermal-conductivity aluminum continuous phase and air for the holes. Numerical predictions are compared to experimental results obtained from carefully controlled experiments.

2. Theoretical models for effective thermal conductivity

We briefly review in this section the most relevant theoretical models (*combined* and *network* type) for effective thermal conductivity, which will be used later in this paper to compare and discuss the numerical results. As mentioned before, Wang and Pan [9] and Churchill [22] have done extensive reviews of theoretical and numerical models. The well-known model due to Krischer [15] (considered a *combined model*) accounts for differences in structure using an empirical weighting factor for the Series and Parallel structures. The value of the weighting parameter must be determined experimentally and cannot be assessed mechanistically from information about the physical structure. Hence, since it is difficult to make a reasonable estimate of the Krischer parameter based on intuition, the use of this model as a prediction tool is very limited. A recent work by Jagjiwanram [14] introduced a *network*-type one-parameter model to predict the ETC for highly porous two-phase systems, where particles of irregular shape have been assumed to be distributed randomly in the continuum. Predictions were compared with experimental results for aluminum–air composites. The temperature was averaged within each phase, and