International Journal of Thermal Sciences 120 (2017) 400–426

Contents lists available at ScienceDirect

International Journal of Thermal Sciences

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

The method of quasiperiodic fields for thermal conduction in periodic heterogeneous media: A theoretical analysis

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ARTICLE INFO

Article history:
Received 24 May 2016
Received in revised form
18 May 2017
Accepted 19 May 2017

Keywords:
Composite material
Thermal conduction
Heat transfer
Upscaling method
Thermal conductivity

ABSTRACT

In this paper, a new theoretical method for upscaling the thermal conduction equation in periodic composite materials is presented. That method is named "the method of quasiperiodic fields", and it is based on the assumption that the temperature field is quasiperiodic at the small scale. More specifically, that method allows to predict the form of the averaged governing equations, and the values of the effective transport coefficients. The new methodology involves four steps: (i) a first level averaging, (ii) the statement of a quasiperiodic problem, (iii) the development of factorized quasiperiodic problems, and (iv) the development of the closed form of the averaged thermal conduction equation. The values of the effective thermal conductivity obtained with that new method were compared with values reported in literature, and also with values obtained from direct numerical simulations.

1. Introduction

Composite materials are encountered in various systems of practical interest, such as hydrogen fuel cells [1], wind turbines [2], car components [3] or civil constructions [4]. However, modeling heat transfer phenomena at the small scale in an entire composite material may be very difficult due to the amount of information that have to be considered. Indeed, solving such problems with numerical simulation software may be impractical, because an extremely fine mesh would be required to capture the local and rapid variations of thermophysical properties in the entire domain of interest. To circumvent this issue, effective thermophysical properties and smoothed governing equations are used to represent heat transfer at the large scale in the materials investigated, which reduces the amount of details required to perform a numerical simulation.

The problem of predicting effective thermal conductivity (ETC) values in composite materials has been addressed by using various methods in the recent literature. A first method consists in using simplifying assumptions about the material structure, which allows to obtain approximate analytical expressions of the ETC value. For example, in Ref. [5], ETC of polymer composites with hybrid filler was estimated by using the law of minimal thermal resistance, and good agreements between theoretical and experimental measured values were obtained. In Ref. [6], the theoretical Maxwell model was improved by taking into account particle-particle contact resistance, which allowed to predict the value of ETC in composite materials. In Ref. [7], the authors highlighted a paradox in the circuit network approach, and they proposed a new statistical model to estimate the value of the ETC in a composite material. In Ref. [8], an approximate analytical model based on equivalent resistances was used to estimate the ETC value of a binary metallic composite. In Ref. [9], new correlations for predicting the ETC value of a nanofluid (water with Carbon nanotubes) was developed, and these correlations agreed within a 5% error band with the values obtained by experimental measurements. In Ref. [10], the rule of mixtures was modified in order to develop an improved expression for predicting ETC in composites, and that new expression provided better predictions than other expressions proposed earlier in literature.

Another method for predicting the ETC value in composite materials consists in performing direct numerical simulations (DNS) in representative volumes of the materials investigated. For example, in Ref. [11], numerical simulations were used to optimize the small scale topology of a composite material and to maximize the value of the effective thermal conductivity. In Ref. [12], local solutions of the periodic conduction problem were obtained within representative volume elements of a composite material by using Green operators, which allowed to calculate the value of the ETC with respect to various geometrical parameters. In Ref. [13], numerical simulations were performed to solve the thermal

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http://dx.doi.org/10.1016/j.ijthermalsci.2017.05.020

Nomenclature

Symbols

a	generic quasiperiodic field
a^{per}	generic periodic field
$\boldsymbol{a}$	source term (vector), °C m^{-1}
$\mathscr{A}_0$	composite material outer boundary
$\mathscr{A}_{0\text{D}}$	part of $\mathscr{A}_0$ dedicated to Dirichlet boundary condition
$\mathscr{A}_{0\text{N}}$	part of $\mathscr{A}_0$ dedicated to Neumann boundary condition
$\mathscr{A}^{\text{AEV}}$	boundary of averaging elementary volume
$\mathscr{A}^{\text{PEV}}$	boundary of periodic elementary volume
$\mathscr{A}^{\alpha i}$	surface repeated along vector $\boldsymbol{\lambda}_i (i = 1, 2, 3)$
$\mathscr{A}^{\alpha i'}$	surface associated $\mathscr{A}^{\alpha i}$
b	source term (scalar), °C
$\boldsymbol{c}$	vector with constant components
$\boldsymbol{I}$	diagonal unit tensor
k	isotropic local thermal conductivity (scalar), W m^{-1} $°\text{C}^{-1}$
k_α	constant thermal conductivity in α phase (scalar), W m^{-1} $°\text{C}^{-1}$
k_β	constant thermal conductivity in β phase (scalar), W m^{-1} $°\text{C}^{-1}$
$\boldsymbol{K}$	local thermal conductivity (tensor), W m^{-1} $°\text{C}^{-1}$
$\mathbb{K}$	effective thermal conductivity (tensor), W m^{-1} $°\text{C}^{-1}$
L_0	composite material characteristic length, m
L^{AEV}	averaging elementary volume characteristic length, m
L^{PEV}	periodic elementary volume characteristic length, m
Δl_1, Δl_2	size of β phase in PEV, m
$\boldsymbol{n}$	outward normal unit vector
$\mathscr{O}$	origin for vectors
r	circle radius of β phase, m
T	temperature field, °C
T_0	temperature value at outer boundary $\mathscr{A}_{0\text{D}}$, °C
$\boldsymbol{T^a}$	factoring field associated to $\boldsymbol{a}$, m
$T_i^{\boldsymbol{a}}$	y_i-component of $\boldsymbol{T^a} (i = 1, 2, 3)$, m
T^b	factoring field associated to b, dimensionless
T^h	factoring field (homogeneous solution), °C
T^{per}	periodic component of temperature field, °C
$\mathscr{V}_0$	composite material domain
$\mathscr{V}^{\text{AEV}}$	domain of averaging elementary volume
$\mathscr{V}^{\text{PEV}}$	domain of periodic elementary volume
V^{AEV}	volume of averaging elementary volume, m^3
V	volume, m^3
v	position along vertical virtual line, m
w	position along horizontal virtual line, m
$\boldsymbol{x}$	vector position, m
x_i	i-component of $\boldsymbol{x}$ $(i = 1, 2, 3)$, m
$\boldsymbol{y}$	vector position, m
y_i	i-component of $\boldsymbol{y}$ $(i = 1, 2, 3)$, m
Δy_1, Δy_2	size of PEV, m
$\langle\rangle$	averaging operator

Greek symbols

ε	scalar vanishingly small
ε_α	volume fraction of α phase in PEV
$\boldsymbol{\lambda}_i$	lattice vector #i $(i = 1, 2, 3)$
ψ	generic variable (scalar, vector, tensor)
$\boldsymbol{\psi}$	generic variable (vector)

Subscripts

$(\boldsymbol{x})$	with respect to position $\boldsymbol{x}$
$(\boldsymbol{y})$	with respect to position $\boldsymbol{y}$

Superscripts

$\hat{\ }$	unit vector
$\overset{\frown}{\ }$	dummy variable
$\tilde{\ }$	deviation field

Abbreviations

AEV	averaging elementary volume
DNS	direct numerical simulation
ETC	effective thermal conductivity
MAH	multiscale asymptotic homogenization
MVA	method of volume averaging

conduction equation in a periodic unit cell representing the composite material, and the resulting ETC values were in good agreement with the experimental results. In Ref. [14], numerical simulations were performed in a representative unit cell to predict the ETC of particle- and fiber-reinforced composites. These numerical results were in good agreement with analytic and approximated solutions obtained by theoretical deduction. In Ref. [15], the authors investigated the performance of heat sink equipment made of phase change materials and of conduction enhancing materials, and the effective thermal conductivity of these composite materials was predicted by performing numerical simulations in periodic unit cells. In Ref. [16], a finite element model was used to simulate conduction heat transfer in plain woven composites; the results allowed to predict the effective thermal conductivity of the composites with respect to porosity and fiber volume.

Various theoretical upscaling strategies have also been used to predict the ETC value in composite materials. For example, the ‘method of volume averaging’ (MVA) consists in applying averaging operators on the local heat transfer governing equation, which yields the correct form of the smoothed governing equation as well as the value of the ETC for composite materials [17]. For instance, in Ref. [18-21], the MVA was used to obtain a theoretical expression for the effective thermal conductivity value in binary composites. The MVA has also been extended to predict values of effective thermophysical properties when additional physical phenomena are involved. For example, in Ref. [22], the MVA was used to obtain the values of the ETC and of the thermal dispersion tensor in a porous medium involving conduction and convection. In Ref. [23], the MVA was used to obtain the smoothed heat transfer governing equations for turbulent flow in porous media; the authors showed that the effective thermal conductivity tensor may be expressed as the sum of a tortuosity tensor, a turbulent tensor, a dispersion tensor, and a turbulent-dispersion tensor.

Another theoretical upscaling strategy named ‘multiscale asymptotic homogenization’ (MAH) method has been used for predicting ETC values in composite materials. That method typically proceeds by expressing the primitive physical field of interest (e.g. temperature) as an asymptotic expansion, and then by associating terms of equal power in the governing equations [24-26]. For example, the MAH method was used to develop theoretical expressions of the ETC value for binary and ternary composites [27], and also for composites with interfacial thermal barriers [28,29]. In Ref. [30], the MAH method was used to predict the