Thermal properties of composite materials: effective conductivity tensor and edge effects

A. Matine¹, N. Boyard¹, P. Cartraud², G. Legrain², Y. Jarny¹

¹Laboratoire de Thermocinétique de NANTES, UMR 6607, CNRS-Université de Nantes, France
²GeM de Nantes, UMR 6183, CNRS-Ecole centrale de Nantes, France
E-mail: abdelghani.matine@univ-nantes.fr

Abstract. The homogenization theory is a powerful approach to determine the effective thermal conductivity tensor of heterogeneous materials such as composites, including thermoset matrix and fibres. Once the effective properties are calculated, they can be used to solve a heat conduction problem on the composite structure at the macroscopic scale. This approach leads to good approximations of both the heat flux and temperature in the interior zone of the structure, however edge effects occur in the vicinity of the domain boundaries. In this paper, following the approach proposed in [10] for elasticity, it is shown how these edge effects can be corrected. Thus an additional asymptotic expansion is introduced, which plays the role of a edge effect term. This expansion tends to zero far from the boundary, and is assumed to decrease exponentially. Moreover, the length of the edge effect region can be determined from the solution of an eigenvalue problem. Numerical examples are considered for a standard multilayered material. The homogenized solutions computed with a finite element software, and corrected with the edge effect terms, are compared to a heterogeneous finite element solution at the microscopic scale. The influences of the thermal contrast and scale factor are illustrated for different kind of boundary conditions.

1. Introduction

Composite materials are most often an innovative technological solution to improve and create more competitive products in many industrial sectors. In leading-edge domains such as aeronautics, the high performances of composites are an undeniable asset. Metals are then gradually substituted with composites in airplane structures. However, even if it has great advantages for mechanical issues, it may lead to some drawbacks regarding heat transfers. Composite materials are actually so insulating compared to metallic ones that rapidly heat confinement issues occur. To predict the thermal environment of airplane structures (and the associated thermo-mechanical behavior) for design purpose, thermal properties and the associated uncertainties of involved orthotropic composite are thus required. Reliable and efficient methods are necessary for their characterization. Two distinct and complementary approaches can be considered for this issue. The first one is experimental and consists in using dedicated devices to measure the effective anisotropic thermal properties of samples (see [2]). The second is a multiscale approach and aims to calculate the effective thermal conductivity tensor from data known at the scale of the composite components. The first studies done within this framework lead to analytical expressions for the macroscopic thermal behavior ([5],[6]). However, they are restricted to composite with simple geometry. In this work, we choose to

Published under licence by IOP Publishing Ltd 1
apply periodic homogenization based on the asymptotic expansion method ([6],[7],[8]).

Thanks to this approach, the initial problem posed on the heterogeneous domain is split in two problems. A microscopic one to solve on the periodic cell which provides the effective thermal properties of the composite [9]. The second is a macroscopic problem, using the effective properties, which enables the determination of homogenized temperature and heat flux fields in the part. This approach leads to good approximations of both the heat flux and temperature in the interior zone of the structure. However edge effects occur in the vicinity of the domain boundaries due to the loss of periodicity. These edge effects are of crucial importance in thermal science for all experimental devices. It is thus mandatory to take them into account, which can be performed within the framework of the asymptotic expansion method, as it has been done in numerous works done in mechanics ([10],[11],[12],[13]). However, as far as we know, only few works ([3],[4]) have addressed edge effects for thermal applications, introducing the concepts of edge effect conductivity and constriction resistance. Within this context, we thus focus on the study of edge effect (or edge effect) problem, following the approach of H. Dumontet [10] for elasticity. We first recall briefly the main results of homogenization based on the asymptotic expansion method and then present the correction of edge effects by introducing edge effect terms. Then we compare the temperature and heat flux fields obtained from the solution of heterogeneous and homogenized problems respectively, in the case of multilayered composite material. The determination of the size of the edge effect is also discussed.

2. Periodic homogenization

2.1. Problem description

Let us consider a multilayered material domain \( \Omega \) bounded on \( \mathbb{R}^2 \) with boundaries \( \partial \Omega = \bigcup_{i=1}^{4} \Gamma_i \) where \( \Gamma_i \) are the boundaries of \( \Omega \) (figure 1(a)). The macroscopic coordinates of a point of \( \Omega \) are denoted \( x = (x_1, x_2) \) in a cartesian system \( \mathbb{R} = (O, e_1, e_2) \). A heat flux \( F \) is imposed on \( \Gamma_1 \) and a Dirichlet condition \( T = 0 \) is imposed on the other boundaries. The volume heat source is denoted by \( f \). The multilayered material has a periodic structure of thin homogeneous and isotropic layers with a thickness \( l/2 \) along \( e_2 \) direction (see figure 1(a)). We denote \( Y \) the periodic cell (figure 1(b)). Note that this cell may be chosen as a 1D domain since the microstructure is invariant in the \( e_1 \) direction, but in the following a 2D periodic cell is considered. The scale factor \( \epsilon = \frac{l}{L} \) represents the ratio between the size of \( Y \) and the size of \( \Omega \). We can thus define the microscopic coordinate system from \( y = \frac{x}{\epsilon} \).

![Diagram](image-url)

**Figure 1.** \( \Omega \)domain and associated periodic cell \( Y \)
We will denote by $T(x)$ and $\phi(x)$ the temperature and heat flux fields in the heterogeneous medium. These fields satisfy the following conduction heat transfer problem in the steady state:

$$
\begin{align*}
\text{div}_x (-\phi(x)) &= f(x) \quad \text{in } \Omega \quad (1) \\
\phi(x) &= K \nabla_x T(x) \quad \text{in } \Omega \quad (2) \\
T(x) &= 0 \quad \text{on } \Gamma_2, \Gamma_3, \Gamma_4 \quad (3) \\
\phi(x) \cdot n &= F(x) \quad \text{on } \Gamma_1 \quad (4)
\end{align*}
$$

where $n$ is the outward unit normal vector, $\nabla_x$ is the Nabla operator defined by $\nabla_x = \left( \frac{\partial}{\partial x_1} \frac{\partial}{\partial x_2} \right)$ and $K(y_1, y_2)$ the heterogeneous thermal conductivity tensor.

### 2.2. Asymptotic expansion method

The parameter $\epsilon$ being small, the asymptotic expansion method is used ([6]). The temperature $T(x)$ is searched under the form:

$$
T(x) = T_0(x,y) + T_1(x,y) \epsilon + T_2(x,y) \epsilon^2 + \ldots \quad (5)
$$

where $T_k(x)$ is the function at the order $k$ of $\epsilon$ and is supposed to be periodic at the microscopic scale.

Applying this method, one can classically show ([6],[8]) that $T_0(x)$ is the solution of a problem posed on the domain $\Omega$ with a homogenized behavior $K^*$ and which involves the average, over the period, of the 0-th order heat flux:

$$
\begin{align*}
\text{div}_x (-\langle \phi^0 \rangle) &= f(x) \quad \text{in } \Omega \quad (6) \\
\langle \phi^0 \rangle &= K^* \nabla_x T^0 \quad \text{in } \Omega \quad (7) \\
T^0(x) &= 0 \quad \text{on } \Gamma_2, \Gamma_3, \Gamma_4 \quad (8) \\
\langle \phi^0 \rangle \cdot n &= F(x) \quad \text{on } \Gamma_1 \quad (9)
\end{align*}
$$

with $\langle \cdot \rangle = \frac{1}{|Y|} \int_Y \cdot dy$ and with the terms of the homogenized tensor $K^*$ which are given by:

$$
K^*_{i,j} = \frac{1}{|Y|} \int_Y K(e_i - \nabla_y w_i) \cdot e_j \, dy \quad (10)
$$

In this expression, $w_{i=1,2}$ are the solutions of the following elementary problems posed on the periodic cell $Y$ (set of equations (11-12)). For more details, the reader can refer to ([6],[8]).

$$
\begin{align*}
\text{div}_y (K(e_i - \nabla_y w_i)) &= 0 \quad \text{in } Y \quad (11) \\
w_i \text{ is periodic} \quad \text{on } \partial Y \quad (12)
\end{align*}
$$

Due to the periodicity of $w_{i=1,2}$, heat flux $\phi^0(x,y)$ is periodic also, which is not valid on the domain boundaries since the periodicity is lost. Therefore, one has edge effects ([10],[11],[12],[13]), which express that $\phi^0(x,y)$ is a poor approximation of $\phi(x,y)$ close to the boundary. We thus propose a method for improving the accuracy of the homogenized solution.
2.3. Method for edge effect correction

The method used in this work has been proposed in ([10]): it consists in introducing an additional term in the asymptotic expansion in the vicinity of the boundary $\Gamma_1$. To avoid corner effects, periodicity conditions are considered on $\Gamma_3$ and $\Gamma_4$. Due to the periodicity in the $e_2$ direction, this additional term is the solution of a problem posed on a semi-infinite domain denoted $G$ and defined by $G = [0, +\infty[ \times ]-l/2, l/2[$ (figure 2).

\[ G = [0, +\infty[ \times ]-l/2, l/2[ \] (figure 2).

**Figure 2.** Definition of the semi-infinite domain $G$

The temperature is now written as follows:

\[ T(x) = T_0(x) + (T^1(x, y) + T_{ee}^1(x, y)) \cdot \epsilon + ... \] (13)

where the edge effect term $T_{ee}^1$ is defined for $x \in \Gamma'$ and $y = (y_1, y_2) \in G$ and is periodic in the $e_2$ direction.

The edge effect formulation is derived from the condition $\phi'(x) \cdot n = F(x)$ which has to be exactly satisfied at 0-th order. $T_{ee}^1$ is found to be under the form:

\[ T_{ee}^1(x, y) = \sum_{j=1}^{2} \frac{\partial T_0}{\partial x_j}(x) \cdot \chi_j(y) \] (14)

with $\chi_j$ solution of the following edge effect problem posed on $G$:

\[
\begin{cases}
\text{div}_y \left( K(y) \nabla_y \chi_j(y) \right) = 0 & \text{in } G \\
K(y) \left( \nabla_y \chi_j(y) \right) \cdot n = -K(y) \left( \epsilon_j + \nabla_y w_j(y) \right) \cdot n + \frac{1}{|\Gamma'|} \int_{\Gamma'} K(y) \left( \epsilon_j + \nabla_y w_j(y) \right) dy \cdot n \text{ on } \Gamma' \text{ periodic in the } e_2 \text{ direction}
\end{cases}
\] (15)

where $T_0$ is the solution of the homogenized problem.

Existence, uniqueness and behavior at infinity of the solution of this problem have already been studied in ([14]).

2.4. Assessment of the size of edge effects

The problem (15)-(17) is posed on a semi-infinite domain, but it can be shown that $\chi_j$ fields decrease exponentially when $y_1$ tends to infinity. Therefore, we assume that $\chi_i(y_1, y_2)$ can be expressed in the following form:

\[ \chi_i(y_1, y_2) = \psi(y_1, y_2) \exp(-\gamma y_1) \] (18)

If $\gamma$ is known, the semi-infinite domain $G$ can be truncated at a length $h = \frac{3}{\gamma}$, provided that homogeneous Dirichlet conditions are added to problem (15)-(17) on the boundary opposite to
In the case where \( K(y_1, y_2) = \begin{pmatrix} k(y_1, y_2) & 0 \\ 0 & k(y_1, y_2) \end{pmatrix} \) is isotropic, the eigenproblem to solve to estimate the depth of edge effect is:

\[
\begin{align*}
\gamma^2 \psi(y_1, y_2) k(y_1, y_2) + \text{div}_y (K \nabla (\psi)) - \gamma \frac{\partial \psi}{\partial y_1} k(y_1, y_2) - \gamma \frac{\partial}{\partial y_1} (k(y_1, y_2) \psi) &= 0 \quad \text{in } \Omega \\
\psi(y_1, y_2) \text{ is continuous at the interfaces} \\
\psi(y_1, y_2) \text{ periodic in the } e_2 \text{ direction}
\end{align*}
\]

The lowest eigenvalue provides an estimation of \( \gamma \) and therefore, the depth of the edge effect.

2.5. Sum up of the methodology of periodic homogenization

Taking into account the edge effect terms, the asymptotic expansions for the temperature and heat flux fields in the structure are described by:

\[
\begin{align*}
T^\epsilon(x) &= T^0(x) + \epsilon \left( (w(y) + \chi(y)) \nabla_x T^0(x) \right) + \ldots \quad \text{in } \Omega \\
\phi^\epsilon(x) &= (K.e_i - \nabla y \chi_i + \nabla_y w_i) e_j \nabla_x T^0(x) + \ldots \quad \text{in } \Omega
\end{align*}
\]

3. Numerical results

3.1. Solution of the edge effect problem

In this study, we use the commercial software COMSOL Multiphysics®. Table (1) provides the thermal and geometrical properties considered for the multilayered material and the boundary condition applied on \( \Gamma' \) to solve the eigenvalue problem (equations (19)-(21)) on \( G \) to estimate the depth of the edge effect.

| \( k_m (W.m^{-1}.K^{-1}) \) | \( k_f (W.m^{-1}.K^{-1}) \) | \( l (mm) \) | \( L (mm) \) | \( f = 0 \) | \( F (W.m^{-2}) \) |
|---|---|---|---|---|---|
| 0.2 | 5 | 1 | 10 | 0 | 2.10^3 |

Figure (3) presents the eigenvector \( \psi \) associated to the lowest eigenvalue \( \gamma = 6277 m^{-1} \). From these results, one can plot the function \( exp(-y_1.\gamma) \) (see figure (4)) to estimate the depth of the edge effect \( h \).

We can thus observe that the exponential decrease makes the field negligible when \( y_1 = 1 \). This means that \( h = l \) is the minimum width value to consider for solving the edge effect problem (equations (15)-(17)) and \( T_{ee}^1 = 0 \) at \( y_1 = h \). \( T_{ee}^1 \) is plotted on figure (4) for a given value of \( x_2 \) (red line plotted on figure (1(a))). The curve also exhibits an exponential decrease with increasing distance from the boundary \( \Gamma_1 \).
The contrast up to a limit \( k \) has no influence on the edge effect size. However, the amplitudes of the conductivity of the second one (Figure 5) for several values of thermal conductivity \( T \) in independent from the contrast. Figures (5(a)) and (5(b)) represent the edge effect terms \( \phi \) and \( \psi \) and \( \text{ee} \).

### 3.2. Influence of the thermal contrast

The influence of this parameter on the depth of the edge effect is studied by solving the set of equations (19)-(21) for several values of thermal conductivity \( k_f \) of a layer, keeping constant the conductivity of the second one \( (k_m = 0.2W.m^{-1}.K^{-1}) \). It is found that the value of \( \gamma \) is independent from the contrast. Figures (5(a)) and (5(b)) represent the edge effect terms \( T_{ee} \) and \( \phi_{ee}.e_1 \) calculated for several values of thermal contrast.

![Figure 3](image3.png)
**Figure 3.** Eigenvector \( \psi \) associated to the lowest eigenvalue \( \gamma \).

![Figure 4](image4.png)
**Figure 4.** Determination of \( h \) and evolution of \( T_{ee} \) along the red line plotted on figure (1(a)).

![Figure 5](image5.png)
(a) Heat flux density \( \phi_{ee}.e_1 \) versus \( y_1 \)
(b) \( T_{ee} \) temperature

**Figure 5.** \( T_{ee}^1 \) and \( \phi_{ee}^0.e_1 \) along the red line plotted on figure (1(a)) for several thermal contrasts \( k_f/k_m \).

Two results are highlighted from these figures. First, the variation of the thermal contrast has no influence on the edge effect size. However, the amplitudes of \( T_{ee}^1 \) and \( \phi_{ee}^0.e_1 \) increase with the contrast up to a limit \( k_f/k_m = 25 \).
3.3. Influence of the scale ratio $\epsilon$

Figures (6(a)) and (6(b)) depicts the evolution of $T_{ee}^1$ and $\phi_{ee}^0 e_1$ along $y_1$ for different values of $\epsilon$. We first observe that the edge effect term $T_{ee}^1$ tend to become negligible when $\epsilon$ decreases, contrary to $\phi_{ee}^0 e_1$ field. These results confirm that the edge effect correction is not necessary for the temperature field when $\epsilon$ is small ($T^0$ is thus a good approximation of $T^\epsilon$). However, this correction has to be applied from the order 0 of $\epsilon$ since heat flux density is sensitive to edge effect even for small values of the scale ratio.

![Graph showing temperature and heat flux density vs. width of the edge effect for different $\epsilon$ values.](image)

**Figure 6.** $T_{ee}^1$ and $\phi_{ee}^0 e_1$ along the red line plotted on figure (1(a)) for several scale ratios.

3.4. Comparison between the heterogeneous and homogeneous fields

![Graph showing heat flux density and temperature vs. abscissa for different fields.](image)

**Figure 7.** Comparison of homogenized and heterogeneous fields along the red line plotted on figure (1(a)).
Heterogeneous and homogenized fields of temperature and heat flux density along a 1D cut presented on figure (1(a)) (red line) are presented in figures (7(a)) and (7(b)) to underline the importance of boundary corrections.

These curves demonstrate that $T_0^0, T_0^0 + \epsilon T_1$ and heat flux density $\phi_0^0, e_1$ are good approximations of $T^0$ and $\phi^0, e_2$ provided that we are sufficiently far from the boundary $\Gamma_1$, at least at a distance equal to the size of the periodic cell. Thus $T^0 + \epsilon (T^1 + T_{ee}^0)$ and $(\phi^0 + \phi_{ee}^0, e_2)$ have to be considered in order to obtain a good approximation of the heterogeneous fields on the domain $\Omega$.

4. Conclusion

An homogenization approach accounting for edge effects has been developed. This method relies on the solutions of three microscopic problems and a macroscopic problem. The microscopic problems provide effective thermal properties, the depth of edge effects and the edge effect solution. The latter can then correct the solution of the homogenized problem at the macroscopic scale. It leads to a good approximation of the solution, even in the vicinity of the boundary. The accuracy of this approach has been shown through numerical results obtained for a multilayered material and a given set of boundary conditions. However the proposed method suffers limitations since each boundary and corner has to be processed separately, inducing the resolution of several edge effect problems. Work is in progress for using Arlequin approach ([15]), which consists in superimposing, close to the boundary, an heterogeneous model to the homogenized one.

References

[1] Degiovanni A 1977 Diffusivité et méthode flash Revue Générale de Thermique 185 420–41
[2] Thomas M, Boyard N, Lefèvre N, Jarny Y and Delaunay D 2010 An experimental device for the simultaneous estimation of the thermal conductivity 3-D tensor and the specific heat of orthotropic composite materials Compos.Sci. Technol 53 5487–98
[3] Fudym O, Batsale J-C and Lecomte D 2004 Heat diffusion at the boundary of stratified media, Homogenized temperature field and thermal constriction Heat and Mass Transfert 47 2437–77
[4] Batsale J.C, Gobbé C and Quintard M 1996 Local non-equilibrium heat transfer in porous media, Recent Research (Developments in Heat Mass and Momentum Transfer) ed Research Sign Post (Trivandrum : India) 1-21
[5] Hashin Z 1983 Analysis of composite materials-a survey J. Appl. Mech 50 481–505
[6] Bornet M Bretheau T Gilormini P 2001 Homogénéisation en mécanique des matériaux 1 (Paris: Hermes Science)
[7] Sanchezhubert J Sanchez-palencia E 1992 Introduction aux méthodes asymptotiques et à l’homogénéisation (Paris : Masson)
[8] Auriault J Boutin C Geindreau C 2009 Homogénéisation de phénomènes couplés en milieu hétérogènes 1 (Paris : Lavoisier)
[9] Thomas M, Boyard N, Perez L, Jarny Y and Delaunay D 2008 Representative volume element of anisotropic unidirectional carbon-epoxy composite with high-fibre volume fraction Compos.Sci. Technol 68 3184–92
[10] Dumontet H 1990 Homogénéisation et effets de bords dans les matériaux composites (thèses d’état de l’université Pierre et Marie Curie Paris 6)
[11] Buannic N and Cartraud P 2001 Higher-order effective modelling of periodic heterogeneous beams -Part 2: Derivation of the proper boundary conditions for the interior asymptotic solution Int. J. of Solids and Structures 38 7163–80
[12] Leguillon D, Marion G, Harry R and Lécuyer F 2001 The onset of delamination at stress-free edges in angle-ply laminates-analysis of two criteria Compos.Sci. Technol 61 377–82
[13] Pruchnicki E 1999 Overall properties of thin hyperelastic plate at finite strain with edge effects using asymptotic method C. R. Acad. Sci. Ser.2B 327 1185–90
[14] Allaire G and Amar M 1999 Boundary layer tails in periodic homogenization ESAIM: Control Optim. and Calc. Var 4 209–43
[15] Rateau G 2003 Méthode Arlequin pour les problèmes mécaniques multi-échelles : Applications à des problèmes de jonction et de fissuration de structures étalées (PhD thesis, Ecole Centrale Paris 6)