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ASYMPTOTIC EVALUATION OF EFFECTIVE TRANSPORT COEFFICIENTS AND LOCAL FIELDS DISTRIBUTIONS IN FIBRE-REINFORCED COMPOSITES

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Abstract. Based on the homogenization method, we propose an asymptotic approach to evaluate effective transport properties of a fibre-reinforced composite material. The cell problem is solved through the shape perturbation technique. The approach is valid for all values of the components' volume fractions and properties. The obtained results are in line with other authors' data.

Introduction. Theoretical prediction of effective transport properties of composite materials is an important problem in science and engineering receiving considerable attention of many authors (for detailed reviews of the subject see [1–4]). In the present paper we shall discuss it with a reference to the heat conductivity, however, all following assumptions also stay true for other transport coefficients such as the electric conductivity, the diffusivity, the dielectric constant, the magnetic permeability and so on. Many of known methods are able to provide accurate numerical results only in certain partial cases of the problem: when volume fraction of one of the components is relatively small (or large), when physical properties of the components are not too distinct, etc. As usual, the main computational difficulties arise when rapid oscillations of physical fields occur in the composite on micro level (e.g., in the case of nearly touching perfectly conductive inclusions). We propose an asymptotic approach which allows to obtain approximate analytical solutions valid for all values of the components' volume fractions and properties.

Our procedure is based on the asymptotic homogenization method [5–9]. The main idea consists in the introduction of two scales of spatial co-ordinates and thus in separating *slow* and *fast* components of the solution. *Slow* components represent changing of physical fields (e.g., temperature) in the composite on macro level, within the whole sample of the material, meanwhile *fast* ones are intended to describe local variations on micro level. Due to the periodicity of the medium *fast* components can be determined from so called cell boundary value problem considered within a distinguished periodically repeatable unit cell of the composite structure. Further application of the volume-integral homogenizing operator allows to establish a link from the micro mechanical response to the behaviour of the material on macro level and to evaluate the effective transport properties. As a rule, the solution of the cell problem presents the main difficulty in practical applications of the homogenization method. Here we develop an approximate analytical solution of the cell problem using the underlying principles of the boundary shape perturbation technique [10].

Governing relations and homogenization procedure: Let us consider steady heat transfer in transverse direction through a fibre-reinforced composite material consisting of a hexagonal array of cylindrical inclusions embedded in an isotropic matrix (Fig. 1); the typical length of heterogeneities l is supposed to be much smaller than the length L of the whole sample of the material ($l << L$). The governing relations can be written in the form of Laplace equations:

$$q^a \left(\frac{\partial^2 T^a}{\partial x_2^2} + \frac{\partial^2 T^a}{\partial x_3^2} \right) = -f, \qquad (1)$$

here and in the sequel variables indexed by "m" correspond to the matrix, indexed by "in" correspond to inclusions, the index "a" takes both of these references $"a" = "m","in"$. In the formula above q^a are the conductivities of the components, T^a is the function of temperature distribution; f is the density of heat sources. The perfect bonding conditions at the components' interface $\partial\Omega$ correspond to the equalities of temperatures and heat fluxes:

$$T^m = T^{in}\Big|_{\partial\Omega}, q^m \frac{\partial T^m}{\partial \mathbf{n}} = q^{in} \frac{\partial T^{in}}{\partial \mathbf{n}}\Bigg|_{\partial\Omega}, \qquad (2)$$

where $\partial/\partial\mathbf{n}$ is the normal derivative to $\partial\Omega$.

We go on to study the input boundary value problem (1), (2) by means of the homogenization method. Let us introduce a natural small parameter

$$\varepsilon = l/L,\ \varepsilon << 1 \qquad (3)$$

characterizing the rate of heterogeneity of the composite structure. Then the scale of co-ordinates is changed. Instead of the original variables x_s,

$s = 1, 2, 3$ we introduce *slow* co-ordinates

$$x_s = x_s \qquad (4)$$

and *fast* ones

$$y_s = x_s \varepsilon^{-1}, \qquad (5)$$

here for the reason of convenience *slow* co-ordinates are denoted by the previous notations x_s. The spatial derivatives are transformed as follows:

$$\frac{\partial}{\partial x_s} = \frac{\partial}{\partial x_s} + \varepsilon^{-1} \frac{\partial}{\partial y_s}. \qquad (6)$$

Slow co-ordinates are used for study of the problem on macro level, within the whole sample of the material. *Fast* ones are intended for the investigation of the composite structure on micro level, within a distinguished unit cell (Fig. 2). This allows to separate slow and fast components of the solution. The length of the side of the unit cell in co-ordinates x_s equals l (Fig. 1), meanwhile in co-ordinates y_s it equals L (Fig. 2).

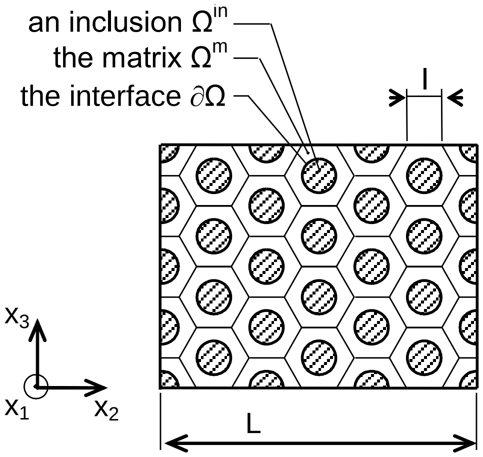


Fig. 1. Composite structure under consideration.

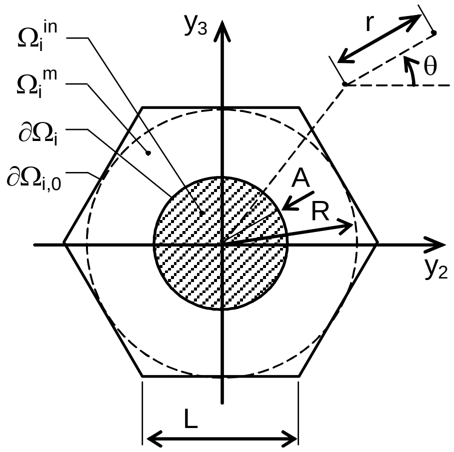


Fig. 2. Periodically repeatable unit cell.

The temperatures T^a are searched as the asymptotic expansions

$$T^a = T_0(x_s) + \varepsilon T_1^a(x_s, y_s) + \varepsilon^2 T_2^a(x_s, y_s) + \ldots. \qquad (7)$$

Here the first term $T_0 = T_0^m = T_0^{in}$ represents the homogeneous component of the temperature field; it changes slowly on the scale of the whole material and does not depend on *fast* variables. All next terms T_i^a, $i = 1,2,3,...$ describe local variations of the temperature on the scale of heterogeneities. The micro periodicity of the medium induces the following periodicity conditions for T_i^a:

$$T_i^a\left(x_s, y_s\right) = T_i^a\left(x_s, y_s + L\right). \tag{8}$$

We substitute relations (4)–(6) and series (7) into the input problem (1), (2). Collecting coefficients at terms of equal powers of ε one comes to a recurrent sequence of boundary value problems:

$$\frac{\partial^2 T_0^a}{\partial y_2^2} + \frac{\partial^2 T_0^a}{\partial y_3^2} = 0, \tag{9}$$

$$T_0^m = T_0^{in}\Big|_{\partial\Omega_i}, \; q^m \frac{\partial T_0^m}{\partial \mathbf{k}} - q^{in}\frac{\partial T_0^{in}}{\partial \mathbf{k}} = 0\Big|_{\partial\Omega_i}; \tag{10}$$

$$\frac{\partial^2 T_1^a}{\partial y_2^2} + \frac{\partial^2 T_1^a}{\partial y_3^2} = 0, \tag{11}$$

$$T_1^m = T_1^{in}\Big|_{\partial\Omega_i}, \; q^m \frac{\partial T_1^m}{\partial \mathbf{k}} - q^{in}\frac{\partial T_1^{in}}{\partial \mathbf{k}} = \left(q^{in} - q^m\right)\frac{\partial u_0}{\partial \mathbf{n}}\Big|_{\partial\Omega_i}; \tag{12}$$

$$\begin{aligned} &q^m\left(\frac{\partial^2 T_0}{\partial x_2^2} + \frac{\partial^2 T_0}{\partial x_3^2} + 2\frac{\partial^2 T_1^m}{\partial x_2 y_2} + 2\frac{\partial^2 T_1^m}{\partial x_3 y_3} + \frac{\partial^2 T_2^m}{\partial y_2^2} + \frac{\partial^2 T_2^m}{\partial y_3^2}\right) + \\ &+q^{in}\left(\frac{\partial^2 T_0}{\partial x_2^2} + \frac{\partial^2 T_0}{\partial x_3^2} + 2\frac{\partial^2 T_1^{in}}{\partial x_2 y_2} + 2\frac{\partial^2 T_1^{in}}{\partial x_3 y_3} + \frac{\partial^2 T_2^{in}}{\partial y_2^2} + \frac{\partial^2 T_2^{in}}{\partial y_3^2}\right) = -f, \end{aligned} \tag{13}$$

$$T_2^m = T_2^{in}\Big|_{\partial\Omega_i}, \; q^m \frac{\partial T_2^m}{\partial \mathbf{k}} - q^{in}\frac{\partial T_2^{in}}{\partial \mathbf{k}} = q^{in}\frac{\partial T_1^{in}}{\partial \mathbf{n}} - q^m \frac{\partial T_1^m}{\partial \mathbf{n}}\Big|_{\partial\Omega_i}; \tag{14}$$

where $\partial\Omega_i$ is the components' interface in the unit cell, $\partial/\partial\mathbf{k}$ is the normal derivative to $\partial\Omega_i$ written in *fast* variables.

The first boundary value problem (9), (10) is satisfied trivially since T_0 does not depend on *fast* co-ordinates ($\partial T_0/\partial y_s = \partial T_0/\partial\mathbf{k} = 0$). Equations (11), (12) define the cell problem, owing to the periodicity of T_1^a by y_s (8) it is considered within only one distinguished unit cell. The solution of the cell problem allows to determine the local variations of the temperature T_1^a. The effective heat conductivity $\langle q\rangle$ can be evaluated from the next boundary value problem (13), (14). Let us apply to equation (13) the homogenizing operator $\iint\limits_{\Omega_i^m}(\cdot)\,dy_2 dy_3 + \iint\limits_{\Omega_i^{in}}(\cdot)\,dy_2 dy_3$. Terms containing T_2^a are eliminated by means of Green's theorem taking into account the boundary conditions (14) and the periodicity relations (8). After routine transformations we obtain

$$\begin{aligned} &\left((1-c)q^m + cq^{in}\right)\left(\frac{\partial^2 T_0}{\partial x_2^2} + \frac{\partial^2 T_0}{\partial x_3^2}\right) + \frac{2q^m}{3\sqrt{3}L^2}\iint\limits_{\Omega_i^m}\left(\frac{\partial^2 T_1^m}{\partial x_2 \partial y_2} + \frac{\partial^2 T_1^m}{\partial x_3 \partial y_3}\right)dy_2 dy_3 + \\ &+\frac{2q^{in}}{3\sqrt{3}L^2}\iint\limits_{\Omega_i^{in}}\left(\frac{\partial^2 T_1^{in}}{\partial x_2 \partial y_2} + \frac{\partial^2 T_1^{in}}{\partial x_3 \partial y_3}\right)dy_2 dy_3 = -f, \end{aligned} \tag{15}$$

where c is the inclusion's volume fraction, $c = 2\pi A^2 \big/ \left(3\sqrt{3}L^2\right) = 0 ... \pi\big/\left(2\sqrt{3}\right)$ Substituting into equation (15) expressions for T_1^a evaluated below we shall come to so called homogenized equation

$$\langle q\rangle\left(\frac{\partial^2 T_0}{\partial x_2^2}+\frac{\partial^2 T_0}{\partial x_3^2}\right)=-f\,, \qquad (16)$$

where the effective conductivity $\langle q\rangle$ can de derived in an explicit analytical form after the evaluation of the integrals in equation (15). However, in the present paper we calculate these integrals numerically in program package *Maple* using standard in-built subroutines.

Solution of the problem: The solution of the cell problem presents one of the main difficulties in practical applications of the homogenization method. Interactions between neighbouring inclusions induce rapid oscillations of the temperature field on micro level. As the inclusions' volume fraction and the contrast between the components' conductivities increase the local temperature gradient can grow significantly, in this case the overall behaviour of the material is strongly governed by the specific geometry of the micro structure. Then many of commonly used methods may face computational difficulties: analytical approaches, which represent distributions of physical fields by various infinite series, can lack convergence and therefore a number of additional terms of the series need to be calculated; the finite elements method can require drastically increase in the density of the discretization mesh; etc. In the present paper we develop an approximate analytical solution of the cell problem valid for all values of the components' volume fractions and properties using the underlying principles of the boundary shape perturbation technique [10]. The basic idea of this approach consists in searching an asymptotic solution of the given boundary value problem in the form of an expansion by a natural small parameter reflecting a discrepancy in shapes between the input domain and a certain relatively simple geometrical figure. The rigorous mathematical justification as well as convergence estimations of the procedure were given by Guz and Nemish [10].

Following the boundary shape perturbation technique we replace in the first approximation the square contour of the outer boundary $\partial\Omega_{i,0}$ of the unit cell by a circle of radius R (Fig. 2), find the solution of the cell problem (8), (11), (12) in polar co-ordinates $r=\sqrt{y_2^2+y_3^2}$, $\theta=\arctan(y_3/y_2)$ assuming $R=\text{const}$ and finally introduce the dependence of the distance R upon the polar angle $R=R(\theta)$ in such a way that to reproduce the original hexagonal shape of the unit cell. The mathematical sense of this simplification is that we satisfy the periodicity and boundary conditions (8), (12) strictly, but involve a certain residual gap into the constitutive equation (11), which is to be compensated in the next approximations. The local variations of the temperature T_1^a are derived as follows:

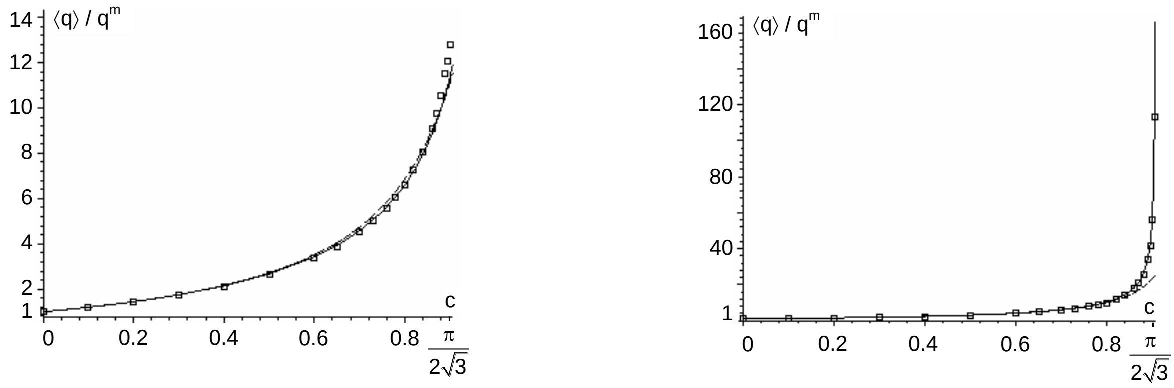
$$T_1^m=\left(C_1 r+C_2 r^{-1}\right)\frac{\partial T_0}{\partial \mathbf{n}},\ T_1^{in}=C_3 r\frac{\partial T_0}{\partial \mathbf{n}}; \qquad (17)$$

$$C_2=-\frac{\lambda\frac{3\sqrt{3}c}{2\pi}L^2}{1-\lambda\frac{2\sqrt{3}c}{\pi}\cos^2(\theta-\alpha)},\ C_3=-\lambda\frac{1-\frac{2\sqrt{3}c}{\pi}\cos^2(\theta-\alpha)}{1-\lambda\frac{2\sqrt{3}c}{\pi}\cos^2(\theta-\alpha)};$$

$$\alpha=\frac{\pi}{6}+\frac{\pi}{3}k\ \text{ at }\ \frac{\pi}{3}k<\theta\le\frac{\pi}{3}(k+1),\ k=0,1,2,\dots.$$

where $\lambda=\left(q^{in}-q^m\right)/\left(q^{in}+q^m\right)$.

Numerical results: In Fig. 3 the developed solution for the effective conductivity $\langle q\rangle$ is compared with results of Perrins et al. [11] and Vanin [12] at different values of the components' properties. Perrins' approach is based on the idea inspired by Lord Rayleigh to describe polarization of each inclusion in an external field by an infinite set of multipole moments. Then corresponding multipole coefficients can be calculated from an infinite set of linear equations. Application of digital computers allows to take into account a large number of multipoles and to improve efficiently the computational accuracy of the method. Vanin's solution consists in a representation of physical fields in the composite by certain complex multi-periodic functions which are further determined by means of series expansions in powers of local co-ordinates. It should be pointed out that both Perrins' and Vanin's methods are not applicable in the limiting case of perfectly conductive nearly touching inclusions ($q^{in}/q^{m}=\infty$, $c\to\pi/\left(2\sqrt{3}\right)$) when rapid oscillations of the temperature field occur on micro level and the magnitude of the effective conductivity with respect to the conductivity of the matrix tends to infinity ($\langle q\rangle/q^{m}\to\infty$). Our approach allows to predict this case correctly.



(a) $q^{in}/q^{m}=20$. **(b)** $q^{in}/q^{m}=\infty$.

Fig. 3. Effective heat conductivity $\langle q\rangle$. Solid curves – present solution, dash curves – results of Vanin [12], boxes – data of Perrins et al. [11].

Conclusions: In the present paper we proposed an asymptotic approach for evaluating the effective transport properties of the fibre-reinforced composite material consisting of the regular hexagonal array of cylindrical inclusions embedded in the isotropic matrix. Our procedure is based on the homogenization method. The cell problem is solved using the underlying principles of the boundary shape perturbation technique. As the results we derive approximate analytical solutions for the effective heat conductivity and for the local distributions of the temperature field. The significant advantage of the developed procedure is that it is applicable for all values of the components' volume fractions and properties. In particular, the obtained solutions work well in cases when rapid oscillations of the temperature occur on micro level (e.g., in the case of perfectly conductive nearly touching inclusions), while many of commonly used methods may face computational difficulties. Extension of the proposed approach to other types of periodic composite structures is a subject to further research.

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