EFFECTIVE THERMAL CONDUCTIVITY OF A MEDIUM WITH ELLIPSOIDAL PARTICLES

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The principal components of the effective thermal conductivity tensor, characterizing stationary heat macrotransfer in a dense medium with dispersed ellipsoidal particles of a different material are calculated by a method suggested in [1]. The case of equally oriented ellipsoids and of isotropically distributed ones are considered as examples.

1. Consider an averagely homogeneous material consisting of a dense medium with thermal conductivity λ_1, containing particles of another substance with thermal conductivity λ_2. The particles are assumed identical, shaped as ellipsoids of revolution of distinct axis **e**. The ellipsoid centers are randomly distributed in space, so that there is no correlation between different positions.

The orientation of the vector **e** is arbitrary with preferred direction **m**. For convenience we identify **m** with the Z axis of the laboratory coordinate system. The position of the coordinate system (x_1, x_2, x_3), fixed in an arbitrary ellipsoid, is given by transformation matrix γ_{ik}, determined in terms of the Euler angles, with **e** in the x_3-axis direction. The angular ensemble distribution function of N particles is

$$f(a_1, \ldots, a_N) = \prod_{i=1}^{N} f(a_i), \qquad \int f(a)\, da = 1$$
$$a = \{\varphi, \psi, \theta\}, \quad da = \sin\theta\, d\varphi\, d\psi\, d\theta \tag{1.1}$$

In the following we denote by angular brackets an ensemble average, and by square brackets an average over a physically small volume containing sufficiently many particles.

The effective thermal conductivity tensor of the material λ_{ik}, characterizing heat macrotransfer in it, has two different principal values and is determined as follows

$$[Q]_i = -\lambda_{ik}[\nabla T], \quad [\mathbf{Q}] = (1-\rho)[\mathbf{Q}_1] + \rho\int f(a)[\mathbf{Q}_2]\, da$$
$$[\nabla T] = (1-\rho)[\nabla T_1] + \rho\int f(a)[\nabla T_2]\, da \tag{1.2}$$
$$[\mathbf{Q}_1] = -\lambda_1[\nabla T_1] = -\lambda_1\nabla\langle T_1\rangle, \qquad [\mathbf{Q}_2] = -\lambda_2[\nabla T_2]$$

where ρ is the bulk concentration, and the indices 1 and 2 refer to the binder and filler, respectively.

2. According to the method discussed in detail in [1], a real particle perturbation is replaced by a perturbation of a point dipole D, applied to the particle center. To determine $[\nabla T_2]$ the thermal conductivity problem in a body with complex geometry is replaced by a thermal conductivity problem in a homogeneous medium with arbitrary embedded ellipsoids.

As can be shown [1], the average temperature satisfies the equation

$$\lambda_1\Delta\langle T_1\rangle = \nabla\mathbf{d}, \qquad \mathbf{d} = \int \mathbf{D}n(a)\, da \tag{2.1}$$

where **d** is the average dipole moment per unit volume, and $n(a) = nf(a)$ is the particle concentration.

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Since the only averagely distinct directions in space are $\nabla\langle T_1\rangle$ and $\mathbf{m}$, it is assumed that

$$\mathbf{d} = \alpha\nabla\langle T_1\rangle + \beta(\nabla\langle T_1\rangle\mathbf{m})\mathbf{m} \tag{2.2}$$

where α, β = const, depending on λ_1, λ_2, ρ, and the particle shape.

Eq. (2.1) is then written in the laboratory coordinate system in the form

$$\begin{gathered}\lambda'(\partial^2/\partial X^2 + \partial^2/\partial Y^2)\langle T_1\rangle + \lambda''(\partial^2/\partial Z^2)\langle T_1\rangle = 0\\ \lambda' = \lambda_1 - \alpha,\ \lambda'' = \lambda_1 - \alpha - \beta\end{gathered} \tag{2.3}$$

To determine α, β consider the effect of an arbitrary embedded ellipsoid on heat transfer in an anisotropic medium (λ', λ'') with constant temperature gradient $\mathbf{E}$ at infinity. The solution of the problem gives an expression for ∇T_2, enabling us to calculate d from Eq. (2.1) and to obtain an equation determining α and β.

In the coordinate system

$$x = X,\ y = Y,\ z = k^{-1}Z,\ k^2 = \lambda''/\lambda'$$

referring to an arbitrary particle center we have outside the ellipsoid Eq. (2.3) and inside and on the boundary

$$\begin{gathered}\lambda'\Delta\langle T_1\rangle = 0\\ \lambda_2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)T_2 + k^{-2}\lambda_2\frac{\partial^2}{\partial z^2}T_2 = 0\\ \langle T_1\rangle = T_2, \qquad \mathbf{n}\mathbf{Q}^{(1)} = \mathbf{n}\mathbf{Q}^{(2)}, \qquad \nabla\langle T_1\rangle \to \mathbf{E}^{(1)}, \qquad \mathbf{r}\to\infty\end{gathered} \tag{2.4}$$

It is well known [2] that the solution of the problem stated satisfies the relations

$$\begin{gathered}E_i^{(2)} - \hat{n}_{ik}(Q_k^{(2)}/\lambda' + E_k^{(2)}) = E_i^{(1)}\\ \mathbf{E}^{(2)} = \nabla T_2, \quad Q_k^{(2)} = -\lambda_k^{(2)}E_k^{(2)}, \quad \lambda_1^{(2)} = \lambda_2^{(2)} = \lambda_2, \quad \lambda_3^{(2)} = k^{-2}\lambda_2\end{gathered} \tag{2.5}$$

where $\mathbf{Q}^{(2)}$ is the heat flow inside the ellipsoid. Transforming to the coordinate system (x, y, z), the ellipsoid with depolarization tensor $n_{ik} = \gamma_{li}\gamma_{lk}n_l$ transforms to an ellipsoid with depolarization tensor $n_{ik} = \Gamma_{li}\Gamma_{lk}n_l$, where n_l are the principal values. The components of the transformation matrix Γ_{ik} to its axes depend on the Euler angles of the new angles, with $\langle\Gamma_{li}\Gamma_{lk}\rangle = 0$, $i \neq k$. We note that the transformation axes of the ellipsoid, and conseqeuntly also n_l, depend on $\cos^2\theta$ and λ''/λ' only.

From Eq. (2.5) we find the temperature gradient $\mathbf{E}^{(2)}$, generated in an ellipsoid inserted in an anisotropic medium with temperature gradient $\mathbf{E}$

$$E_i^{(2)} = N_{ik}E_k,\ N_{ik}^{-1} = \delta_{ik} + \hat{n}_{ik}(\lambda_s^{(2)}/\lambda' - 1) \tag{2.6}$$

In the laboratory coordinate system we calculate the dipole moment $\mathbf{D}$ and $\mathbf{d}$ from Eq. (2.1)

$$\begin{gathered}\mathbf{D} = \int(\mathbf{q}n)\,\mathbf{r}ds, \qquad \mathbf{q} = -\lambda_2\mathbf{E}^{(2)} + \lambda_1\mathbf{E}\\ D_i = V(\lambda_1\delta_{ik} - \lambda_2N_{ik})E_k,\ d_i = \rho(\lambda_1\delta_{ik} - \lambda_2\langle N_{ik}\rangle)E_k\end{gathered} \tag{2.7}$$

where V is the ellipsoid volume. It can be shown that

$$\langle N_{ik}\rangle = 0,\ i \neq k,\ \langle N_{11}\rangle = \langle N_{22}\rangle$$

Comparing Eqs. (2.2) and (2.7), we obtain equations determining α and β as functions of ρ, λ_1, λ_2, n_l

$$\begin{gathered}\alpha = \rho(\lambda_1 - \lambda_2\langle N_{11}\rangle),\ \alpha = \lambda_1 - \lambda'\\ \alpha + \beta = \rho(\lambda_1 - \lambda_2\langle N_{33}\rangle),\ \alpha + \beta = \lambda_1 - \lambda''\end{gathered} \tag{2.8}$$

3. The effective thermal conductivity λ_{ik} is calculated from Eq. (1.2). By (2.6) and (2.8) the average heat flow and average temperature gradient are

$$\begin{gathered}[Q]_i = -\{(1-\rho)\lambda_1 + \rho\lambda_2\langle N_{ii}\rangle\}\nabla\langle T_1\rangle = \begin{cases}-\lambda'\nabla\langle T_1\rangle;\ i = 1, 2\\ -\lambda''\nabla\langle T_1\rangle;\ i = 3\end{cases}\\ [\nabla T]_i = (1 - \rho + \rho\langle N_{ii}\rangle)\nabla\langle T_1\rangle\end{gathered} \tag{3.1}$$

In the dimensionless variables

$$\varkappa = \lambda_2/\lambda_1,\ \xi_1 = \xi_2 = \lambda'/\lambda_1,\ \xi_3 = \lambda''/\lambda_1,\ \Lambda_{ik} = \lambda_{ik}/\lambda_1$$

the principal components Λ_i of the effective thermal conductivity tensor Λ_{ik} are:

in the preferred directions of ellipsoid orientation

$$\Lambda_3 = \xi_3 (1 - \rho + \rho\langle N_{33}\rangle)^{-1} \tag{3.2}$$

in any direction perpendicular to it

$$\Lambda_1 = \Lambda_2 = \xi_1 (1 - \rho + \rho\langle N_{11}\rangle)^{-1} \tag{3.3}$$

where $\langle N_{ii}\rangle$ is evaluated by Eq. (2.6) and Eqs. (2.8), determining λ', λ''.

When the distant ellipsoid axes are parallel [the angular distribution function being $f(a) = {}^1/{}_2\,\pi^{-2}\delta(\cos\theta - 1)$]

$$\begin{aligned}\langle N_{33}\rangle &= \{1 + \hat{n}_3 (\lambda_2 / \lambda' - 1)\}^{-1}\\ \langle N_{11}\rangle = \langle N_{22}\rangle &= \{1 + n_1 (\lambda_2 / \lambda' - 1)\}^{-1}\end{aligned} \tag{3.4}$$

From Eqs. (3.2) and (3.3) the principal values of the effective thermal conductivity tensor are

$$\begin{aligned}\Lambda_3 &= \xi_3 \{\xi_3 (1 - \hat{n}) + \varkappa\hat{n}\} \{(1 - \hat{n} + \rho\hat{n})\xi_3 - \varkappa\hat{n}(1 - \rho)\}^{-1}\\ \Lambda_1 &= \xi_1 \{\xi_1 (1 + \hat{n}) + \varkappa (1 - \hat{n})\} \{(1 + \hat{n} + \rho (1 - \hat{n}))\, \xi_1 - \varkappa (1 - \hat{n})(1 - \rho)\}^{-1}\\ \hat{n} &= \hat{n}_3\end{aligned} \tag{3.5}$$

It is somewhat complicated to calculate ξ_i from Eq. (2.8) and $\hat{n} = \hat{n}(\xi_3/\xi_1)$, the depolarization coefficient in the transformed coordinate system [see Eq. (2.4)].

For an isotropic angular distribution function $f(a) = 1/8\pi^{-2}$ the effective thermal conductivity tensor is spherical. Denoting the depolarization coefficient n_3 by n ($n_1 = n_2 = (1-n)/2$) and taking into account that

$$N_{ik} = \gamma_{li}\gamma_{lk} \{1 + n_l (\lambda_2 / \lambda' - 1)\}^{-1},\ \langle\gamma_{li}^2\rangle = {}^1/{}_3$$

we obtain from Eq. (2.8) a cubic equation for $\xi = \lambda'/\lambda_1$

$$\begin{aligned}&\xi^3 (1 - n^2) + \xi^2 \{\varkappa (1 - n + 2n^2) - \rho\varkappa ({}^5/{}_3 - n) - (1 -\\ &- \rho)(1 - n^2)\} + \xi\varkappa \{\varkappa n (1 - n) - \rho\varkappa (n + 1/3) - (1 - \rho)(1 - n + 2n^2)\} - \varkappa^2 n (1 - n)(1 - \rho) = 0\end{aligned} \tag{3.6}$$

The coefficients are such that only one positive root is possible. Based on Eqs. (3.2), (3.3), and (3.6), the dimensionless effective thermal conductivity of the material is

$$\begin{aligned}\Lambda &= \lambda / \lambda_1 = \xi\Delta \{(1 - \rho)\Delta + \rho\xi^2 ({}^5/{}_3 - n) + \rho\xi\varkappa (n + {}^1/{}_3)\}^{-1}\\ \Delta &= \xi^2 (1 - n^2) + \xi\varkappa (1 - n + 2n^2) + \varkappa^2 n (1 - n)\end{aligned} \tag{3.7}$$

For fixed ρ $\varkappa < 1$ the quantity Λ has a maximum at n = 1/3, corresponding to spherical particles. If $\varkappa > 1$, Λ is minimum at n = 1/3. The spherical embedding was considered in detail in [1]. Fig. 1 shows the dependence of Λ on log $\varkappa$ at $\rho = 0.1$ (dotted line), and at $\rho = 0.3$ (full time). The curves 1 correspond to r lens shape (n = 0.9), and curves 2 to a needle shape (n = 0.5). Curves 3 (n = 1/3), lying for $\varkappa < 1$ above, and for $\varkappa > 1$ below the corresponding curves 1, 2, characterize the model of "overlapping" spheres [1].

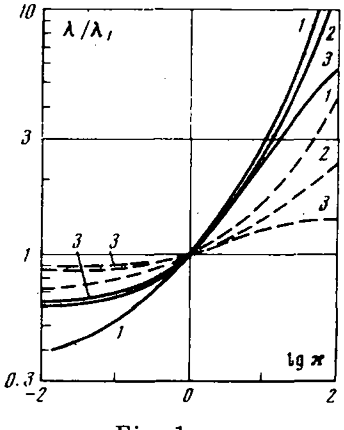

Fig. 1

We stress that the equations obtained are applicable to sufficiently small ρ, since the distribution function of particle centers used achieves particle overlap in space at high bulk concentrations ρ. Therefore, obviously, ξ in Eq. (3.6) and the effective thermal conductivity Λ in Eq. (3.7) become infinite at $\varkappa \to \infty$ and $\rho > \rho_*$, $\rho_* = n(1-n)/(n+1/3)$ (max $\rho_* = 1/3$ is also reached for n = 1/3).

For spherical embedding it is possible to introduce (see [1]) a distribution function of centers, taking into account that particles do not overlap. Comparison of results for the models of "overlapping" and "nonoverlapping" spheres showed that the values of effective thermal conductivity Λ are close for $\rho < \rho^* = 1/3$ and $\varkappa \leqslant 10$.

We note that the corresponding problems of determining the effective thermal conductivity, the dielectric function, and the electric conductivity are mathematically equivalent.

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LITERATURE CITED

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