METHOD OF INTEGRAL CROSS SECTIONS IN HEAT CONDUCTION PROBLEMS

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We substantiate estimates of the upper and lower bounds of the effective thermal conductivity of piecewise homogeneous bodies. A numerical scheme for calculating the temperature field has been developed and implemented, and a comparison between the results of calculations by different schemes has been carried out.

Introduction. At the present time a number of methods are available that permit one to investigate various physical properties of composite materials with a complex form of inclusion [1-3]: however, each method has its advantages and disadvantages. For example, use of the method of averaging is hampered by the complexities of the asymptotic solution and the means of constructing it [2, p. 21]. At the same time, the available methods are universal, provide possibilities for a unified approach to a number of seemingly diverse problems, and permit one to take into account end offects and the geometry of the inhomogeneities.

The present article is devoted to a further investigation of the method of integral cross sections, which is simple to implement and makes it possible not only to calculate the effective characteristics of composites but also to calculate the local temperature and mechanical fields by taking into account the shape of the inclusion and the properties of the interaction between the matrix and the inclusion of a microinhomogeneous material.

The method of cross sections was used for the first time by Rayleigh for determining the effective conductivity λ [4], and subsequently it was developed in [5-8, etc.]. The estimates of the upper and lower bounds of λ obtained in those works were substantiated by proceeding from general physical considerations rather than rigorously. Therefore, we shall first obtain estimates of the upper and lower bounds of λ by means of the method of integral cross sections, and then we shall give basic results obtained within the framework of this approach.

In [8-13] estimates of the upper and lower bounds of λ are given that were obtained on the basis of variational methods. For this purpose, the authors of [9] invoked the principle of minimum entropy production:

$$\frac{dS}{d\tau} = -\int \int \int \frac{\nabla t \mathbf{q}}{T} dV \ge 0.$$
⁽¹⁾

According to Eq. (1), the integral (the dissipation of energy during passage of the heat flux q)

$$I = \frac{1}{2V} \int \int_{(V)} \int \mathbf{q}(\mathbf{r}) \,\nabla t(\mathbf{r}) \,dx_1 \,dx_2 \,dx_3 \tag{2}$$

subject to the additional condition

$$\operatorname{div}\left(\mathbf{q}\left(\mathbf{r}\right)\right)=0\tag{3}$$

is stationary and takes a minimum value ($\delta J = 0$) on the class of admissible functions q(r), $\nabla t(r)$ that satisfy the equations

div
$$(\lambda (\mathbf{r}) \nabla t (\mathbf{r})) = 0$$
, $\mathbf{q} (\mathbf{r}) = -\lambda (\mathbf{r}) \nabla t (\mathbf{r})$. (4)

For convenience in further formulations we shall introduce the operators of averaging over the coordinates:

$$\left\{f\left(\mathbf{r}\right)\right\}_{L} = \frac{1}{L} \int_{0}^{L} f\left(\mathbf{r}\right) dx_{k}, \quad \left\{f\left(\mathbf{r}\right)\right\}_{S} = \frac{1}{S} \iint_{(S)} f\left(\mathbf{r}\right) dx_{i} dx_{j}.$$

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Fig. 1. Structure of a microinhomogeneous material: a) representative volume; b) differential volumetric element (DVE) in the form of a prism; c) DVE in the form of a layer.

In this case, the following equalities are satisfied:

$$\left\{ \left\{ f(\mathbf{r}) \right\}_{S} \right\}_{L} = \left\{ \left\{ f(\mathbf{r}) \right\}_{L} \right\}_{S} = \left\langle f(\mathbf{r}) \right\rangle.$$

Estimates of Upper and Lower Bounds. Hill proved [14] that for a quasihomogeneous body the following equality holds:

$$\langle \mathbf{q} (\mathbf{r}) \nabla t (\mathbf{r}) \rangle = \langle \mathbf{q} \rangle \langle \nabla t \rangle,$$
 (5)

where $\langle \mathbf{q} \rangle = -\lambda \langle \nabla t \rangle$.

Theorem. If $\delta \iiint_{(V)} \lambda(\mathbf{r}) (\nabla t)(\mathbf{r})^2 dV = 0$ on the class of admissible functions $q(\mathbf{r}), \nabla t(\mathbf{r})$ satisfying the equations div $(\lambda(\mathbf{r})\nabla t(\mathbf{r})) = 0, q(\mathbf{r}) = -\lambda(\mathbf{r})\nabla t(\mathbf{r})$ and $\langle q(\mathbf{r})\nabla t(\mathbf{r}) \rangle = \langle q \rangle \langle \nabla t \rangle$, then

$$\left\{ \left\{ \lambda^{-1} \right\}_{L}^{-1} \right\}_{S} \leq \lambda \leq \left\{ \left\{ \lambda \right\}_{S}^{-1} \right\}_{L}^{-1}.$$
(6)

Proof. On the basis of Eqs. (2)-(4) we conclude that any other choice of the pair of functions q'(r), $\nabla t(r)$ or q(r), $\nabla t'(r)$ from the class of admissible functions that satisfy the boundary conditions, just like the true functions q(r), $\nabla t(r)$, gives a value of J' such that the following condition holds:

$$I' \ge J, \tag{7}$$

where

$$J^{'} = -\langle \mathbf{q}^{'} \nabla t \rangle, \quad \langle \mathbf{q}^{'} \rangle = -\lambda^{'} \langle \nabla t \rangle,$$

or

 $J^{'} = -\langle \mathbf{q} \nabla t^{'} \rangle, \quad \langle \nabla t^{'} \rangle = -\rho \langle \mathbf{q} \rangle.$

Here λ' and ρ' are quantities that determine the effective properties of fictitious bodies (bodies of comparison) that are characterized by the pairs of functions q'(r), $\nabla t(r)$ and q(r), $\nabla t'(r)$, respectively.

We present two techniques for selecting the trial functions q'(r) and $\nabla t'(r)$ that permit one to find the upper and lower bounds for the effective thermal conductivity of microinhomogeneous materials. The estimates of the upper and lower bounds obtained by means of the method of integral cross sections are based on two techniques of arbitraty division of a representative volume V. In one case it (Fig. 1a) is divided in the chosen direction (along the external field), for example, along the $0x_3$ axis, into prisms with area of the base $dx_1 \times dx_2$ and height L (Fig. 1b), and in the other case – into layers of thickness dx_3 with area of the base $L \times L$ (Fig. 1c).

Let us prove the right-hand side of inequality (6). We represent the expression for the flux $\langle q \rangle$ in the form

$$\langle \mathbf{q} \rangle = -\left\{ \left(\left\{ \lambda \left(\mathbf{r} \right) \nabla t \left(\mathbf{r} \right) \right\}_{S} \right) \right\}_{L}.$$
 (8)

we now select the trial functions $q'(\mathbf{r})$, $\nabla t(\mathbf{r})$ in such a way that the following condition is satisfied:

$$\left\{ \mathbf{q}'\left(\mathbf{r}\right) \right\}_{S} = \left\langle \mathbf{q}' \right\rangle. \tag{9}$$

The term inside the round brackets in Eq. (8) determines the mean flux q over the cross section of the specimen; subject to condition (9) it can be determined in the form

$$\left\{\lambda\left(\mathbf{r}\right)\nabla t\left(\mathbf{r}\right)\right\}_{S}=\left\{\lambda\right\}_{S}\left\{\nabla t\left(\mathbf{r}\right)\right\}_{S}.$$
(10)

Here $\{\lambda\}_S = \lambda_1 \overline{S}_1(x_3) + \lambda_2 \overline{S}_2(x_3)$ is the conductivity of a layer of thickness dx_3 ; S is the cross-sectional area of the generalized representative element (GRE) perpendicular to the $0x_3$ axis; $S_l(x_3)$ is the cross-sectional area of the specimen perpendicular to the $0x_3$ axis and occupied by the *l*-th component (l = 1, 2):

$$S = S_1(x_3) + S_2(x_3), \quad \overline{S}_l(x_3) - S_l(x_3)/S.$$

From Eq. (10) it follows that

$$\langle \nabla t \rangle = -\left\{ \left\{ \lambda \right\}_{S}^{-1} \right\}_{L} \langle \mathbf{q}' \rangle.$$

Taking into account the fact that $-\langle q \rangle \langle \nabla t \rangle \leq -\langle q' \rangle \langle \nabla t \rangle$, we obtain an upper bound for λ :

$$\lambda \leq \left\{ \left\{ \lambda \right\}_{S}^{-1} \right\}_{L}^{-1}.$$
⁽¹¹⁾

Now, in order to prove the left-hand side of inequality (6), we represent $\langle \nabla t \rangle$ in the form

$$\langle \nabla t \rangle = \left\{ \left(\left\{ \nabla t \left(\mathbf{r} \right) \right\}_{L} \right) \right\}_{S}.$$
 (12)

We select the trial functions $\nabla t'(\mathbf{r})$, $\mathbf{q}(\mathbf{r})$ in such a way that the following relation is satisfied:

$$\left\{ \nabla t' \left(\mathbf{r} \right) \right\}_{L} = \left\langle \nabla t' \right\rangle.$$
⁽¹³⁾

With account for Eq. (13) the integral within the round brackets in Eq. (12) can be represented in the form

$$\left\{ \nabla t'(\mathbf{r}) \right\}_{L} = -\left\{ \lambda^{-1} \right\}_{L} \left\{ \mathbf{q}(\mathbf{r}) \right\}_{L}, \qquad (14)$$

where $\{\lambda^{-1}\}_L$ is the resistance of a prism of height L with area of the base $dx_1 dx_2$. In this case

$$\left\{\lambda^{-1}\right\}_{L} = \overline{L}_{1}(x_{1}, x_{2})\lambda_{1}^{-1} + \overline{L}_{2}(x_{1}, x_{2})\lambda_{2}^{-1}.$$

Here $L_l(x_1, x_2)$ is the length of the straight line that is parallel to the $0x_3$ axis and passes along the *l*-th component $(l = 1, 2); \overline{L_l(x_1, x_2)} = L_l(x_1, x_2)/L$ is the length of the GRE along the $0x_3$ axis.

From Eq. (14) we obtain

$$\langle \mathbf{q} \rangle = -\left\{ \left\{ \lambda^{-1} \right\}_{L}^{-1} \right\}_{S} \langle \nabla t' \rangle$$

Thus

$$J' = 1/2 \langle \mathbf{q} \rangle \langle \nabla t' \rangle = 1/2 \left\{ \left\{ \lambda^{-1} \right\}_{L}^{-1} \right\}_{S} \langle \mathbf{q} \rangle^{2}.$$
⁽¹⁵⁾

Taking into account Eq. (15) and the fact that

$$J = 1/2 \langle \mathbf{q} \rangle \langle \nabla t \rangle = -1/2 \lambda^{-1} \langle \mathbf{q} \rangle^2, \qquad (16)$$

according to Eq. (7), for the effective conductivity λ of the microinhomogeneous material we can write

$$\lambda \ge \left\{ \left\{ \lambda^{-1} \right\}_{L}^{-1} \right\}_{S}.$$
⁽¹⁷⁾



Fig. 2. Plane network of randomly distributed resistances: a) initial; b) subject to condition (10); c) subject to condition (14).

Combining Eqs. (11) and (17), we obtain bounds of possible values for the effective conductivity in the form

 $\left\{\left\{\lambda^{-1}\right\}_{L}^{-1}\right\}_{S} \leq \lambda \leq \left\{\left\{\lambda\right\}_{S}^{-1}\right\}_{L}^{-1},$

which was to be proved.

In [2] it was concluded that in the case of equal volumetric fractions of the inclusion and the matrix the effective coefficient of thermal conductivity differs from the mean arithmetic and the mean harmonic coefficients of the inclusion and the matrix; moreover, the greater the difference between the thermal conductivity coefficient of the inclusion and that of the matrix, the greater the difference between the effective coefficient of thermal conductivity and the indicated mean values. In our case we have proved the theorem about an accurate estimation of the boundaries of the change in the effective coefficient of thermal conductivity.

Inequality (6) is equivalent to the following well-known rule: the true value of the effective conductivity λ is higher than the conductivity obtained in the case of an "adiabatic" cross section and lower than that obtained in the case of an "isothermal" cross section of a piecewise composite body.

To illustrate the physical meaning of assumptions (10) and (14), let us consider the plane network of two types of randomly distributed resistances depicted in Fig. 2. To estimate the upper bound of the effective resistance of such a network, we assume that all of the transverse connections are broken (Fig. 2b). This is equivalent to assumption (10). It is clear that such an assumption should lead to an overestimation of the effective resistance (lowering of the conductivity), since the finite resistances were replaced by infinite ones (discontinuities), i.e., the new network of resistances will have a lower conductivity than the initial one. To estimate the lower bound, we will assume that all of the transverse resistances are equal to zero (Fig. 2c); this is equivalent to assumption (14). With such a replacement the effective resistance will be underestimated compared to the resistance of the initial network, and the conductivity will be correspondingly overestimated.

The method of cross sections in one form or another was used by many authors to determine the effective conductivity [4-8]. We will present some of the results without giving derivations. For an elementary cell of a sphere in a cube, using Eq. (6), we can represent the lower and upper bounds as follows:

the lower bound

$$\lambda_{\text{low}} = \lambda_2 + (\lambda - \lambda_2) \pi_2,$$

$$\pi_2 = \pi^{1/3} (3\varphi_1/4)^{2/3},$$

$$\tilde{\lambda} = \frac{2\lambda_2}{(a-1)\pi_1} \left\{ 1 - \frac{1}{(a-1)\pi_1} \ln [(a-1)\pi_1 + 1] \right\},$$

$$\pi_1 = 2 (3\varphi_1/4\pi)^{1/3},$$

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where $a = \lambda_2/\lambda_1$, λ_2 and λ_1 are the conductivity of the matrix and the inclusion, respectively; φ_1 is the volumetric concentration of the inclusion: $\varphi_1 = V_1/V$, V_1 is the volume of the inclusion, V is the volume of the matrix;

the upper bound

$$\lambda_{\rm up} = \left(\frac{1-\pi_1}{\lambda_2} + \frac{\pi_1}{\lambda_{\rm c.s}}\right)^{-1},$$

$$\lambda_{\rm c.s} = \lambda_2 (1-a^{-1}) \pi_2 \left[J_p(1)\right]^{-1}, \quad P = 1 + \frac{a}{(1-a)\pi_2}$$

$$J_{\rm up}(z) = \begin{cases} \frac{1}{2\sqrt{b}} \ln \frac{z-\sqrt{b}}{z+\sqrt{b}}, & b > 0, \\ \frac{1}{\sqrt{|b|}} \arctan \frac{z}{\sqrt{|b|}}, & b < 0. \end{cases}$$

For an elementary cell of a cube in a cube the lower and upper bounds have the form [4]

$$\lambda_{\text{low}} = \lambda_2 \, \frac{\lambda_1 - (\lambda_1 - \lambda_2) \, (1 - \varphi_1^{2/3}) \, \varphi_1^{1/3}}{\lambda_1 - \varphi_1^{1/3} \, (\lambda_1 - \lambda_2)}, \tag{18a}$$

$$\lambda_{\rm up} = \lambda_2 \, \frac{\lambda_2 + (\lambda_1 - \lambda_2) \, \varphi_1^{2/3}}{\lambda_2 + (\lambda_1 - \lambda_2) \, \varphi_1^{2/3} \, (1 - \varphi_1^{1/3})} \,. \tag{18b}$$

Thus, the sequence for determining the lower bound for the effective properties of the conductivity of a microinhomogeneous material is as follows: first, the piecewise homogeneous body is split into differential volumetric elements in the form of prisms, and averaging of the properties along the chosen direction (along the external field) is done, and then (finally) averaging is done over the cross section perpendicular to the chosen direction (perpendicular to the external field). The upper bound for the effective properties of the conductivity is determined in a different sequence: first the averaging is done over the cross section perpendicular to the chosen direction and only then along the chosen direction. Obviously, a combined method can be used. In this case the piecewise homogeneous body is arbitrarily divided into two regions: in one of these the determination of the effective properties is made using the formulas for the lower bound, and in the other – using the formulas for the upper bound. Then, performing the averaging of the properties over these two regions, we obtain formulas for the effective properties of the whole piecewise homogeneous body, a calculation by means of which gives values lying within the bounds of the possible values obtained from Eq. (6).

Numerical Scheme of Calculation. We will consider the construction of a finite-difference scheme by means of the method of integral cross sections concerning the calculation of the temperature field in the following problem:

$$Lu = \operatorname{div} \lambda(r) \nabla u(r) = \begin{cases} L_1 u = \operatorname{div} (\lambda_1 \nabla u_1(r)) = 0, & \text{if } r \in D_1, \\ L_2 u = \operatorname{div} (\lambda_2 \nabla u_2(r)) = 0, & \text{if } r \in D_2, \end{cases}$$
(19)

where *u* is the potential in the region $D = D_1 \cup D_2$. At the phase interface $B = D_1 \cap D_2$ the following conditions are fulfilled:

$$\mathbf{q}_i = -\lambda_i \, \nabla u_i \,, \quad i = 1 \,, \, 2 \,.$$

Here **n** is the unit normal vector to B, $\mathbf{q}_i = -\lambda_i \nabla u_i$, i = 1, 2.

We will construct the finite-difference scheme for Lu = 0 in the following way. By means of the planes $x_i = kh$ (k = 1, 2, ..., n) we construct a rectangular grid B_n that splits the region D into $(n-1)^{\alpha}$ cubes $(\alpha$ is the dimensionality of the region D). There will be three types of cubes:

1) consisting only of component 1, i.e., having the volume $V_{1k} < D_1$ (conductivity $\lambda_{kn}^{(1)}$);

2) consisting only of component 2, i.e., having the volume $V_{2k} < D_2$ (conductivity $\lambda_{kn}^{(2)}$);



Fig. 3. Effective thermal conductivity of an elementary cell of a cube in a cube: 1) calculation by formula (18b); 2) numerical calculation; 3) calculation by formula (18a).

3) consisting of components 1 and 2, i.e., having the volume $V_{3k} > B$ (conductivity $\lambda_{kk}^{(3)}$).

Then, we replace each cube by a node (the node is located at the center of the cube) with six connections that are determined by the conductivities of the cube in three directions.

The conductivity of connections between neighboring nodes that belong to different types of cubes is determined as the harmonic mean of the conductivities of these cubes in the given direction. For example, the conductivity of the connection (l, l+1) is equal to

$$\lambda_{l,l+1} = \left\{ 1/2 \left[\left(\lambda_l^{(i)} \right)^{-1} + \left(\lambda_{l+1}^{(3)} \right)^{-1} \right] \right\}^{-1}, \quad i = 1, 2.$$

Here, $\lambda_l^{(i)}$ and $\lambda_{l+1}^{(3)}$ are the conductivities of the cubes in the *l*-th direction whose centers are located at the nodes M_{lmn} and $M_{l+1,m,n}$. In this case $\lambda_{kk}^{(3)}$ is determined by means of the method of integral cross sections.

The boundary conditions and the conditions of the interaction of the matrix with the inclusion are taken into account by selecting the properties (in a given case, the conductivity) of the connections between neighboring nodes of the computational scheme. The conductivity of a connection can both take a specific value and be determined as a function of a certain coefficient of interaction, for example, the coefficient of resistance between the matrix and the inclusion.

As a result of such a construction, we obtain a new grid B_n' whose nodes M_{lmn} are joined by three types of connections. The approximation of the derivatives $u(\mathbf{r})$ in Eq. (19) takes the form

$$\lambda (\mathbf{r}) \frac{\partial u (\mathbf{r})}{\partial x_1} = \frac{\lambda_{l,l+1}}{h} (u (l+1, m, n) - u (l, m, n)),$$

$$\frac{\partial}{\partial x_1} \left(\lambda (\mathbf{r}) \frac{\partial u (\mathbf{r})}{\partial x_1}\right) = \frac{1}{2h^2} \left[\lambda_{l+1,l}^{(n,m)} u (l+1, m, n) - (\lambda_{l,l-1}^{(n,m)} + \lambda_{l+1,l}^{(n,m)}) u (l, m, n) + \lambda_{l,l-1}^{(n,m)} u (l-1, m, n)\right].$$

The remaining terms in Eq. (19) are determined in a similar fashion:

$$\frac{\partial}{\partial x_2} \left(\lambda \left(\mathbf{r} \right) \frac{\partial u \left(\mathbf{r} \right)}{\partial x_2} \right) \quad \text{and} \quad \frac{\partial}{\partial x_3} \left(\lambda \left(\mathbf{r} \right) \frac{\partial u \left(\mathbf{r} \right)}{\partial x_3} \right).$$
$$\lambda_{\text{low}} < \lambda_{\text{ef}} < \lambda_{\text{up}} ,$$

The difference scheme used is very efficient, since it has a three-diagonal matrix.

The finite-difference approximation considered has been implemented on a computer. The calculation of one version on an ES-1066 computer takes 30-40 sec. Without limiting the generality, the method of integral cross



Fig. 4. Dependence of the relative temperature $T/\Delta T$ on the coordinates z and y (m): a) thermal conductivity of the matrix $\lambda_2 = 1$ W/(m·deg), thermal conductivity of the inclusion $\lambda_1 = 100$ W/(m·deg); b) $\lambda_2 = 100$ W/(m·deg), $\lambda_1 = 1$ W/(m·deg); ΔT (deg) is the absolute difference of temperatures between the faces of the cube z = 0 and z = h (h = 1.8 m); 1) calculation by the finite-element method; 2) calculation by the method of integral cross sections; 3) a quasihomogeneous medium with $\lambda_{ef} = (1/2) (\lambda_{low} + \lambda_{up})$.

sections permits the solution of the problem for any form of the inclusion with smooth boundaries. This permits one to carry out the integration in formula (6), which gives estimates of the upper and lower bounds of the effective coefficient of thermal conductivity. Thus, the method of integral cross sections makes it possible to circumvent the difficulties in describing the boundary between the various structures of composite materials and can be introduced efficaciously into engineering and other calculations.

As a model structure for determining the effective thermal conductivity we selected an elementary cell a cube in a cube with a ratio of the linear dimensions of 1.8/1 and boundary conditions of the first kind.

Results of Calculation. Using the results of a numerical calculation by the proposed scheme we determined the effective thermal conductivity λ_{ef} of an elementary cell of a cube in a cube (Fig. 3). From a comparison it is seen that λ_{ef} takes values located between the lower and upper bounds of the thermal conductivity coefficient: $\lambda_{low} < \lambda_{ef} < \lambda_{up}$, where λ_{low} and λ_{up} were calculated using formulas (18).

Graphs of the dependence of $T/\Delta T$ on the coordinates z and y for $\lambda_1 = 100$, $\lambda_2 = 1$ and for $\lambda_1 = 1$, $\lambda_2 = 100$ are presented in Fig. 4. It should be noted that, owing to symmetry, the dependence of $T/\Delta T$ on x is completely equivalent to the dependence of $T/\Delta T$ on y.

A comparison of the obtained results with calculations by the finite-element method showed good agreement between them. In Fig. 4 curves 3 differ substantially from curves 1 and 2. This indicates that in calculating the temperature field of a piecewise homogeneous body, its replacement by a quasihomogeneous medium with the effective thermal conductivity $\lambda_{ef} = (1/2) (\lambda_{low} + \lambda_{up})$ leads to a substantial error. Conclusions. Estimates of the upper and lower bounds for the effective thermal conductivity of piecewise homogeneous bodies have been substantiated. A numerical method for calculating the temperature fields in piecewise homogeneous bodies has been developed and implemented that agrees well with the finite-element method and is simple in implementation.

NOTATION

S, area; τ , time; V, volume; t, T, temperature; q, vector of the heat flux density; λ , effective generalized conductivity; r, radius vector; ∇ , gradient; div, divergence; ρ , density of a substance; L, length; ΔT , temperature drop. Subscripts: low, lower; up, upper; ef, effective.

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