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THERMAL CONDUCTIVITY AND QUASIHOMOGENEITY CRITERION OF DISPERSE MATERIALS

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We suggest a method of numerical calculation of the effective thermal conductivity and the time for establishing quasihomogeneity of disperse materials. The method is based on the principle of generalized conductivity realizable within the framework of a nonstationary thermal problem.

Calculation of the thermal conductivity of disperse materials is usually based on the principle of generalized conductivity. According to this principle, the structure of the material is modeled using its most simplified element, i.e., a unit cell. The considered heat exchange in a unit cell must reflect the most essential features of heat exchange in the material itself. Calculation of heat exchange to determine the effective thermal conductivity is carried out within the framework of a stationary thermal problem. Additional conditions such as the adiabaticity of the side surfaces of the cell and isothermicity of its end-face surfaces are superimposed on the heat exchange (see Fig. 1).

The calculation scheme suggested below presupposes the use of a nonstationary thermal problem for determining the heat exchange in a unit cell. For this purpose, following the recommendations given in [1], the type of unit cell is selected. It is assumed that the cell is in contact with a semibounded homogeneous medium with an effective thermal conductivity calculated for the given type of cell by the method of [2]. The heat capacity of the medium is determined by an additive scheme. The side surfaces of the unit cell are adiabatic, and the thermal power $Q = \int qdS$ (q = const) is liberated on the lower horizontal surface, i.e., a boundary condition of the second kind is prescribed. Then, a nonstationary thermal problem is solved with account for the boundary conditions on the surfaces S_1 and S_2 with the initial conditions $t = 0$ and $T = 0$. A numerical calculation makes it possible to determine $q(x, y, z = 1)$ and $Q = \int qdS$ on the surface S_2. At a certain instant of time $t = \tau$ the quantity $Q(x, y, z = 0)$ becomes equal to $Q(x, y, z = 1)$ with a certain proportionality factor k whose choice is determined by the specific material and the aims of the calculation carried out. The time τ is identified with the period of establishment of a quasistationary process; when $t < \tau$ the disperse sample is not quasihomogeneous. At the time τ the mean temperatures of the surfaces $T_1 = \int_{S_1} TdS$ and $T_2 = \int_{S_2} TdS$ and their difference $\Delta T = T_2 - T_1$ are determined, and then the effective thermal conductivity of the disperse medium is found:

$$\lambda_{\text{ef}} = \frac{kqSl}{\Delta T} . \quad (1)$$

Though being extremely laborious, the above approach has certain advantages over the traditional one. In particular, its use gives additional, fundamentally important information on the time for establishing quasihomogeneity of the material. As regards the calculation of the thermal conductivity itself of the disperse material, the method considered removes the rather artificial requirement of isothermicity for the end faces of the unit cell. We will use this method to calculate the characteristics of the simplest (lamellar) systems.

Layers Perpendicular to the Heat Flux. We consider a lamellar material consisting of N substances. Their layers, repeated periodically, comprise the structure of the material. We know the values of the coefficients of

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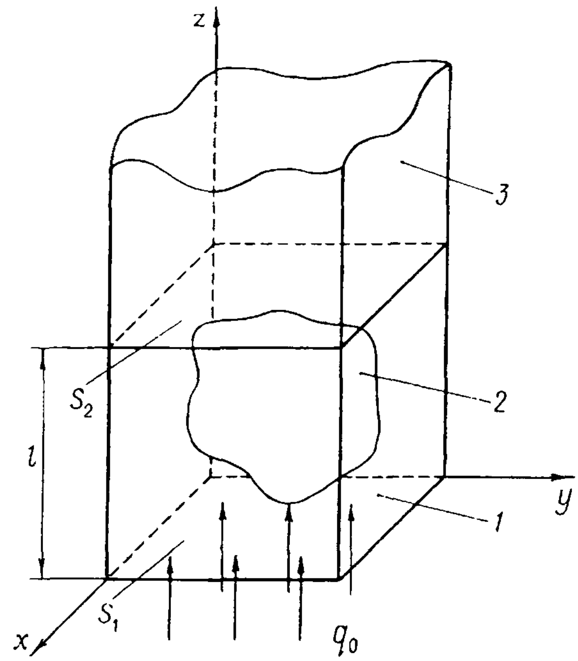

Fig. 1. Example of a unit cell: 1 and 2) first and second components, 3) quasihomogeneous semi-infinite medium.

density, heat capacity, and thermal conductivity and the volumetric concentrations for each of the substances; the thickness of the layers is $l_1, \ldots, l_N$. In the present case the adiabatic surfaces are perpendicular to the layers of the material, and consequently, we may use a one-dimensional approximation scheme. As the unit cell, it is advisable to take the first group of layers 1, ..., N (see Fig. 2a). We replace the remaining portion of the material by a quasihomogeneous medium $N+1$.

The temperature field of such a system is described by the system of equations

$$\frac{\partial^2 T_m}{\partial x^2} = \frac{1}{a_m}\frac{\partial T_m}{\partial t}, \quad m = 1, \ldots, N+1, \tag{2}$$

with the initial condition

$$T_m(x, 0) = 0, \quad m = 1, \ldots, N+1, \tag{3}$$

and the boundary conditions

$$-\lambda_1 \left.\frac{\partial T_1}{\partial x}\right|_{x=0} = q_0, \tag{4}$$

$$T_{N+1}(x = \infty, t) = 0. \tag{5}$$

We assume that on the interfaces between the media S_m the following conditions are satisfied:

$$T_m|_{x\in S_m} = T_{m+1}|_{x\in S_m}, \quad \lambda_m \left.\frac{\partial T_m}{\partial x}\right|_{x\in S_m} = \lambda_{m+1}\left.\frac{\partial T_{m+1}}{\partial x}\right|_{x\in S_m}, \quad m = 1, \ldots, N. \tag{6}$$

For the quasihomogeneous medium $N+1$, we can calculate the values of the thermal conductivity and thermal diffusivity coefficients.

The thermal conductivity coefficient is defined by the relation

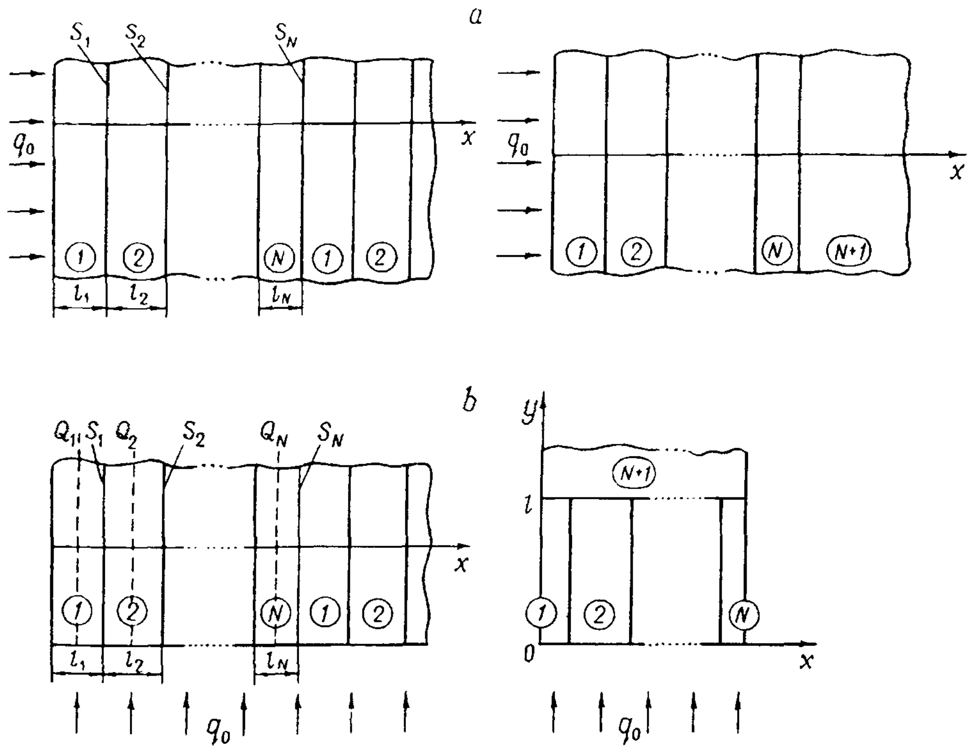

Fig. 2. Layers perpendicular (a) and parallel (b) to the heat flux: 1, 2, ... , N, numbers of the layers; $N+1$, a quasihomogeneous semi-infinite medium.

$$\frac{1}{\lambda_{\text{ef}}} = \sum_{m=1}^{N} \frac{d_m}{\lambda_m}, \tag{7}$$

where d_m is the volumetric concentration of the substance in the material, equal to

$$d_m = \frac{l_m}{\sum_{i=1}^{N} l_i}, \tag{8}$$

where l_m is the layer thickness.

The value of the volumetric heat capacity coefficient is determined from the formula

$$(\rho c)_{\text{ef}} = \sum_{m=1}^{N} d_m \rho_m c_m . \tag{9}$$

The coefficient of effective thermal diffusivity of layer $N+1$ is defined by the relation

$$a_{\text{ef}} = \frac{\lambda_{\text{ef}}}{(\rho c)_{\text{ef}}} . \tag{10}$$

The proposed method makes it possible to evaluate the time for establishing quasihomogeneity. We solve the problem of nonstationary heat conduction iteratively and find the heat flux q at the point $x = x_N$. The condition for termination of the iteration process is

$$\frac{(q_0 - q)}{q_0} < \eta , \tag{11}$$

TABLE 1. Results of Numerical Calculation (the thickness of the layers l_i = 1 mm; i = 1, 2, 3; l = 3 mm)

Substances composing the layers	Time required to establish quasihomogeneity τ, sec	Thermal conductivity coefficient λ_{ef}, W/(m·K)	
		exact value	estimated value
Layers perpendicular to the heat flux			
Al	0.7	237.00	238.60
Pb	2.7	35.00	35.23
Al, Cu, Pb	1.72	85.00	84.83
Fe. Cu, Ni	1.86	115.43	116.45
Pb, Cu, Ni	1.98	71.33	71.77
BeO, MgO, Al_2O_3	2.51	66.74	67.21
Layers parallel to the heat flux			
Al	0.7	237.00	238.01
Pb	2.7	35.00	35.23
Fe	3.37	80.00	80.54
Pb, Fe, Ni	1.06	67.67	67.82
Pb, Fe, Sn	0.81	60.67	61.28
SiO_2, MgO. Al_2O_3	0.78	37.43	38.51

Note: The values of the coefficients are considered at T = 300 K.

where η is the prescribed error. The time τ for establishing quasihomogeneity of the sample is determined by condition (11). Using formula (1), we calculate the coefficient of effective thermal conductivity, which can be compared with the value obtained from formula (7).

Numerical solution was carried out for three layers (N = 3) for different materials and combinations of them. Results of the calculation are presented in Table 1.

Layers Parallel to the Heat Flux. We consider a lamellar material of N components. The values of the coefficients of density, thermal conductivity, and heat capacity for each component are known. The thickness of the layers $l_1, ..., l_N$ is also given.

It is evident that in the present case the planes Q_m passing through the middle of each layer are adiabatic surfaces (see Fig. 2b). As the unit cell it is natural here to select a portion of the material enclosed between the planes Q_1 and Q_N. We also prescribe the length l. The remaining portion of the material enclosed between the planes Q_1 and Q_N and lying from l to ∞ is replaced by a quasihomogeneous semibounded medium. The temperature field of such a system is described by the equations

$$\frac{\partial^2 T_m}{\partial x^2} + \frac{\partial^2 T_m}{\partial y^2} = \frac{1}{a_m} \frac{\partial T_m}{\partial t}, \quad m = 1, \dots, N + 1, \tag{12}$$

with the initial condition

$$T_m(x, y, 0) = 0, \quad m = 1, \dots, N + 1, \tag{13}$$

and the boundary conditions

$$-\lambda_m \frac{\partial T_m}{\partial y}\Big|_{y=0} = q_0 , \quad m = 1 , \dots , N , \tag{14}$$

$$T_{N+1} (x , y = \infty , t) = 0 . \tag{15}$$

In the given case the equalities of the temperatures at the boundaries of contact of the layers and the equalities of the heat fluxes through the boundaries are

$$T_m|_{x\in S_m} = T_{m+1}|_{x\in S_m} , \quad \lambda_m \frac{\partial T_m}{\partial x}\Big|_{x\in S_m} = \lambda_{m+1} \frac{\partial T_{m+1}}{\partial x}\Big|_{x\in S_m} , \quad m = 1 , \dots , N-1 . \tag{16}$$

$$T_m|_{y\in S_{N+1}} = T_{N+1}|_{y\in S_{N+1}} , \quad \lambda_m \frac{\partial T_m}{\partial y}\Big|_{y\in S_{N+1}} = \lambda_{N+1} \frac{\partial T_{N+1}}{\partial y}\Big|_{y\in S_{N+1}} , \quad m = 1 , \dots , N , \tag{17}$$

$$\frac{\partial T_1}{\partial x}\Big|_{x=0} , \quad \frac{\partial T_N}{\partial x}\Big|_{x\in S_N} = 0 . \tag{18}$$

For calculating the effective value of the thermal conductivity coefficient the following relation is used:

$$\lambda_{\text{ef}} = \sum_{m=1}^{N} d_m \lambda_m , \tag{19}$$

where

$$d_m = \frac{l_m}{\sum_{i=1}^{N} l_i} . \tag{20}$$

The coefficient of volumetric heat capacity is determined by the relation

$$(\rho c)_{\text{ef}} = \sum_{m=1}^{N} d_m \rho_m c_m . \tag{21}$$

The value of the effective thermal diffusivity coefficient of layer $N+1$ is determined in the form

$$a_{\text{ef}} = \frac{\lambda_{\text{ef}}}{(\rho c)_{\text{ef}}} . \tag{22}$$

For solving the two-dimensional problem we use the method of alternating directions [3]. The region is divided parallel to the coordinate axes (a rectangular grid); when the y or x coordinate is fixed on the grid, the corresponding second derivative in the heat conduction equations of system (12) is equated to zero. Thus, we obtain systems of equations involving a single space variable. The overall system is solved by fixing the values of x and y alternately and solving the corresponding set of one-dimensional subproblems on segments and semi-lines. The semi-lines are replaced by segments of sufficient length (the length is selected so that the temperature field has no time to spread to the end of the segment during the time of the the scheme operation). The junction regions of the division where the thermal conductivity and thermal diffusivity coefficients undergo a discontinuity are cut out; here the temperature values are calculated from equations of joining and boundary conditions (16)-(18) using the calculated temperature values on neighboring parallel segments. The scheme is stable and gives an error of the order of the decomposition step.

Similarly to the case of layers perpendicular to the heat flux, we solve the problem of nonstationary heat conduction iteratively, determine the heat flux q through the plane $y = l$, and check the fulfillment of condition (11). From this we find the time after which the material may be considered quasihomogeneous. We also determine the value of the thermal conductivity coefficient from formula (1).

Results of numerical calculation for various combinations of materials are presented in Table 1.

Thus, the method suggested makes it possible to calculate numerically the thermal conductivity coefficients of disperse materials. The structure of the material is modeled by a unit cell with averaged thermophysical coefficients that comes in contact with (borders on) a semibounded body. The method described is based on solution of a nonstationary thermal problem that makes it possible to determine simultaneously both the effective thermal conductivity of the disperse material and the time needed to establish its quasihomogeneity.

NOTATION

a, thermal diffusivity; c, heat capacity; d_m, volumetric concentration of the m-th layer of substance in the material; l, length of the unit cell; q, heat flux density; q_0, constant value of the heat flux density; Q, thermal power; S, area; t, time; T, temperature; T_0, initial temperature; x, y, space coordinates; λ, thermal conductivity coefficient; η, error in the heat flux density; τ, time required to establish quasihomogeneity.

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