The boundary temperatures and the input data for the solution of the inverse problem were the temperatures obtained from the solution of the forward heat-conduction problem for boundary conditions of the second kind and a given thermal conductivity coefficient $\lambda(T) = 0.5 + 2T^2$. The remaining input data were chosen as follows: $q_1 = 1$, $q_2 = 0$, $C(T) = 1$, $b = 1$, $d = 0.5$, and $\tau_m = 1$.

In the spline approximation of the required function $\lambda(T)$ we made three divisions of the temperature interval $[T_{min}, T_{max}]$. The calculations were carried out on the difference net $n_x \times n_\tau = 20 \times 20$. For the 25 iterations we needed about 5 min of the processor time of the computer BÉSM-6. In this example, the problem was solved using exact data. The starting approximation for the heat-conduction coefficient was taken as a constant, and equal to $\lambda_0 = 0.75$. The obtained results demonstrate the sufficiently high efficiency of the suggested algorithm.

NOTATION

T, temperature; C(T), volume heat capacity; $\lambda(T)$, thermal conductivity coefficient; x, d, and X, coordinates; τ, time; b, right-hand boundary along x; τ_m, duration of the process; $f_i(\tau)$, input temperatures; $\vartheta(x, \tau)$, temperature increment; λ_k, $k = 1, 0, \ldots, m + 1$, parameters in the spline approximation of the function $\lambda(T)$; B(T), B spline; α and β, parameters of the conjugate gradients method; J', gradient of the total functional; $\psi(x, \tau)$, conjugate variable; δ^2, integrated error of the input data; and p, number of iterations.

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CONDUCTIVITY OF MULTICOMPONENT HETEROGENEOUS SYSTEMS

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A method is proposed for calculating conductivity of a multicomponent heterogeneous system, taking account of its structure.

The conductivity Λ of a heterogeneous system is the coefficient in the linear relation between the average flux $\langle\vec{j}\rangle$ and the average value of the gradient $\langle\nabla\vec{\varphi}\rangle$ producing it:

$$\langle \vec{j} \rangle = -\Lambda \langle \nabla\vec{\varphi} \rangle, \quad \langle \nabla\vec{\varphi} \rangle = \frac{1}{V}\int_V \nabla\vec{\varphi}_i dV_i. \tag{1}$$

For local regions occupied by the i-th component the following relations are valid:

$$\vec{j}_i = -\Lambda_i \nabla\vec{\varphi}_i, \quad \operatorname{div}\vec{j}_i = 0. \tag{2}$$

Methods of calculating the conductivity of two-component heterogeneous systems as a function of the conductivities of the components Λ_i and their volume concentrations have been developed in adequate detail [1, 2].

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Several formulas are available in the literature for calculating Λ of multicomponent heterogeneous systems. However, analysis showed that all these have faults which prevent their use in calculating the conductivity of these systems with a different structure over a wide range of variation of parameters. Let us discuss the most widely used formulas for Λ.

A formula for Λ based on the "effective medium" model has been derived [3-6] for the effective conductivity of statistical mixtures

$$\sum_{i=1}^{n} \frac{\Lambda_i - \Lambda}{\Lambda_i + 2\Lambda} m_i = 0. \tag{3}$$

We note the fundamental flaws of the "effective medium" model: according to (1), for $\Lambda_1/\Lambda_i = 0$ and $m_1 > 0.7$, we obtain $\Lambda < 0$, which is physically meaningless; for $\Lambda_1/\Lambda_i < 10^{-2}$ there is a poor agreement with experimental data [7, 8]; Eq. (3) is valid only for mixtures of isometric particles, and is an equation of the n-th degree for Λ.

For a mixture of n components with conductivities which are not too different from one another, a relation for Λ has been derived in the form [9]

$$\Lambda^{1/3} = \sum_{i=1}^{n} m_i \Lambda_i^{1/3},$$

which is insensitive to the structure of the mixture.

The Lichtenecker formula [10] derived by the "construction" method is sometimes used to calculate Λ of an n-component mixture:

$$\Lambda = \Lambda_1^{m_1} \Lambda_2^{m_2} \Lambda_3^{m_3} \ldots \Lambda_n^{m_n}.$$

Analysis of Lichtenecker's paper [1, 11] showed that he did not take account of the effect of the structure of the heterogeneous system on the effective conductivity. In addition, if the conductivity of one of the components is zero, the conductivity of the whole system $\Lambda = 0$, which is not true for all structures.

Using the idea of the "construction" method, Novikov [12] proposed the following formula for calculating Λ:

$$\Lambda^k = \Lambda_1^k m_1 + \sum_{i=2}^{n} \Lambda_i^k m_i, \quad \Lambda_1 > \Lambda_i, \quad k = (1 + m_1^{-1/3})^{-1},$$

which also is insensitive to the structure of the mixture.

It was proposed in [1] to determine the conductivity of multicomponent heterogeneous systems by a method which differs from all the preceding proposals in taking account of the structure of a heterogeneous system. The essence of this calculation consists in a step-by-step reduction of a multicomponent system to a two-component system. However, it turned out that the final result of the calculation, i.e., the value of Λ, depended on the sequence in which the reduction to a two-component medium was performed. This raised doubts about the possibility of using this method over a wide range of variation of parameters.

In 1976 Yu. P. Zarichnyak proposed to calculate the conductivity of a two-component heterogeneous structure with a random distribution of components by using the familiar formula for flat tissue structures with an ordered distribution of components [1]

$$\Lambda = \Lambda_1 m_1^2 + 4 m_1 m_2 \frac{\Lambda_1 \Lambda_2}{\Lambda_1 + \Lambda_2} + \Lambda_2 m_2^2. \tag{4}$$

This formula was generalized to a heterogeneous system with n components:

$$\Lambda = \sum_{i=1}^{n} \Lambda_i m_i^2 + 4 \sum_{\substack{i=1 \\ i \neq j}}^{n} m_i m_j \frac{\Lambda_i \Lambda_j}{\Lambda_i + \Lambda_j}. \tag{5}$$

The following assumptions were made in deriving (5): the particles are modeled by cubes with the cubes so disposed that planes passing through the edges of a cube do not intersect other cubes; the heterogeneous system consists of two layers; vertical planes passing through the edges of a cube are adiabatic, i.e., the spatial distribution of the flux is modeled by one-dimensional flow.

Justifying the use of Eq. (5) to calculate the conductivity of a real three-dimensional heterogeneous system consisting of a large number of layers and having a different structure requires special investigations.

Thus, at the present time there is no sufficiently all-purpose procedure for calculating the effective conductivity of multicomponent heterogeneous systems which takes account of the structure of the system.

We describe a method for calculating the conductivity of multicomponent systems which takes account of their structure.

Without loss of generality, we consider first a two-component system with a flux $\vec{j}_i$ through the i-th component. Then, according to (1), we have for the average flux $\langle\vec{j}\rangle$

$$\langle \vec{j} \rangle = \frac{1}{V} \int\limits_{V} \vec{j}_i dV_i = \frac{1}{V} \left[\int\limits_{V_1} \vec{j}_1 dV_1 + \int\limits_{V_2} \vec{j}_2 dV_2 \right]. \quad (6)$$

Substituting the value of $\vec{j}_i$ from (2) into (6):

$$\langle \vec{j} \rangle = -\frac{1}{V} \left[\int\limits_{V_1} \Lambda_1 \vec{\nabla\varphi}_1 dV_1 + \int\limits_{V_2} \Lambda_2 \vec{\nabla\varphi}_2 dV_2 \right] = (-\Lambda_1 m_1 \langle \vec{\nabla\varphi}_1 \rangle + \Lambda_2 m_2 \langle \vec{\nabla\varphi}_2 \rangle), \quad (7)$$

$$\langle \vec{\Delta\varphi}_i \rangle = \frac{1}{V_i} \int\limits_{V_i} \vec{\nabla\varphi}_i dV_i, \ m_i = V_i/V. \quad (8)$$

It follows from (1) and (8) that

$$\langle \vec{\nabla\varphi} \rangle = m_1 \langle \vec{\nabla\varphi}_1 \rangle + m_2 \langle \vec{\nabla\varphi}_2 \rangle. \quad (9)$$

Taking account of (1), we write Eqs. (7) and (9) in the form

$$\Lambda = \Lambda_1 m_1 \Psi_1 + \Lambda_2 m_2 \Psi_2, \quad (10)$$

$$m_1\Psi_1 + m_2\Psi_2 = 1, \ \Psi_i = \langle \nabla\varphi_i \rangle / \langle \nabla\varphi \rangle, \ i = 1, 2. \quad (11)$$

The two equations (10) and (11) contain three unknowns Λ, Ψ_1, and Ψ_2, and therefore further information is necessary, for example, on the structure of the heterogeneous system under study. It is easy to generalize Eq. (10) for an n-component system:

$$\Lambda = \sum_{i=1}^{n} \Lambda_i m_i \Psi_i, \ \sum_{i=1}^{n} m_i \Psi_i = 1. \quad (12)$$

The quantity Ψ_i depends on the structure of the system and the conductivities of the components, and its determination is the basic problem in the analytic determination of the effective conductivity of heterogeneous systems. The quantities Ψ_i are found by constructing models of two-component systems having various structures. Therefore, we try to reduce the problem of determining Ψ_i for a multicomponent system to the problem of finding Ψ_i for a two-component system — a problem which has already been solved.

We single out the i-th component in an n-component system. It will be surrounded by a medium with an effective conductivity $\langle\Lambda_{n-i}\rangle$, which depends on the conductivities of the remaining n − 1 components and their relative positions.

At this time we do not discuss the method of determining $\langle\Lambda_{n-i}\rangle$. We select the conductivity of the i-th component as a basis, denote the conductivity of the whole system by

Λ_i', and rewrite Eq. (12) in the form

$$\Lambda_i' = \Lambda_i m_i \Psi_i + \langle \Lambda_{n-i} \rangle (1 - m_i) \Psi_{n-i}^*, \tag{13}$$

$$m_i \Psi_i + (1 - m_i) \Psi_{n-i}^* = 1, \quad \Psi_{n-i}^* = \langle \nabla \varphi_{n-i}^* \rangle / \langle \nabla \varphi \rangle, \tag{14}$$

where $\langle \nabla \varphi_{n-i}^* \rangle$ is the average potential gradient in the region occupied by the (n − i) components.

Taking account of (14), we can rewrite Eq. (13) in the form

$$\Lambda_i' = \langle \Lambda_{n-i} \rangle + (\Lambda_i - \langle \Lambda_{n-i} \rangle) m_i \Psi_i. \tag{15}$$

Substituting Ψ_{n-i}^* from the first of Eqs. (14) into (13), we obtain

$$m_i \Psi_i = \frac{\Lambda_i' - \langle \Lambda_{n-i} \rangle}{\Lambda_i - \langle \Lambda_{n-i} \rangle}. \tag{16}$$

Equation (12) for the conductivity of multicomponent systems now takes the form

$$\Lambda = \sum_{i=1}^{n} \Lambda_i \frac{\Lambda_i' - \langle \Lambda_{n-i} \rangle}{\Lambda_i - \langle \Lambda_{n-i} \rangle}. \tag{17}$$

We now discuss briefly the determination of the effective conductivity $\langle \Lambda_{n-i} \rangle$ of the system which surrounds the i-th component.

Let us consider, e.g., a three-component system. We single out the i-th component (i = 1, 2, 3). The system surrounding the i-th component is a two-component system. We determine $\langle \Lambda_{n-i} \rangle$ by using the formulas corresponding to the structure of the given two-component system, after renormalizing the volume concentrations of the n − 1 components to unity. If it is difficult to establish the structure of the two-component system, the simplest assumption is made that it is a layered system with the components arranged parallel to the heat flux. We find in succession the three values $\langle \Lambda_{3-1} \rangle$, $\langle \Lambda_{3-2} \rangle$, $\langle \Lambda_{3-3} \rangle$, then the three values Λ_1', Λ_2', Λ_3', and then from Eq. (17) the value of Λ.

This method of calculating the effective conductivity of multicomponent systems can be called self-consistent, since it leads to agreement of the distribution of the potential gradient in each component with all the remaining components for an approximate calculation of the effective conductivity Λ_i'.

Thus, the effective thermal conductivity of multicomponent systems is calculated in three stages. In the first stage the thermal conductivity of the medium surrounding the i-th component is computed by using the formulas describing heat transfer in a layered medium with components parallel to the heat flux:

$$\langle \Lambda_{n-i} \rangle = \sum_{\substack{j=1 \\ j \neq i}}^{n} \Lambda_j m_j', \tag{18}$$

where the m_j' are the volume concentrations of the components renormalized to unity:

$$m_j' = m_j \Big/ \sum_{\substack{k=1 \\ k \neq i}}^{n} m_k, \quad j = 1, 2, \ldots, i-1, i+1, \ldots, n. \tag{19}$$

In the second stage we find the thermal conductivity Λ_i' of the two-component system consisting of the i-th component with a thermal conductivity Λ_i and a concentration m_i and the second component with the thermal conductivity $\langle \Lambda_{n-i} \rangle$ and the volume concentration $1 - m_i$. At this stage it is necessary to take account of the structure of the mixture, viz.: how component i is oriented relative to the remaining "effective" medium. In the third stage the effective thermal conductivity of the whole system is determined by Eq. (17).

As an example, let us consider the calculation of the thermal conductivity of a three-component system in which the first component has a thermal conductivity $\Lambda_1 = 1$ and a volume concentration $m_1 = 0.6$; the second has $\Lambda_2 = 10$ and $m_2 = 0.1$; the third has $\Lambda_3 = 1000$ and

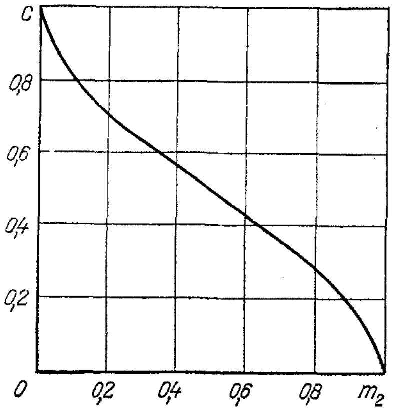

Fig. 1. Parameter c as a function of volume concentration.

TABLE 1. Thermal Conductivity of Three-Component System with Interpenetrating Components

m_1	m_3	Model 1	Model 2	Model 3	Model 4	Model 5
1	2	3	4	5	6	7
0	0,9	670	670	670	670	670
0,1	0,8	516,9	507,8	515,5	501,4	500,4
0,2	0,7	417,3	410,4	411,3	401,9	400,0
0,3	0,6	335,4	325,3	326,8	335,2	333,4
0,4	0,5	260,4	250,3	254,8	252,3	250,0
0,5	0,4	195,3	195,3	191,9	187,4	188,1
0,6	0,3	140,5	140,3	127,4	132,4	130,0
0,7	0,2	89,4	85,4	86,1	82,2	81,6
0,8	0,1	40,9	40,3	41,4	38,7	36,9
0,9	0	1,4	1,4	1,4	1,4	1,4

m_3 = 0.3. The first and second components are distributed in the third: the first in the form of isolated disseminations, and the second in the form of filaments.

In the first stage we use Eq. (18) to determine $\langle\Lambda_{n-i}\rangle$, where i = 1, 2, 3. To do this we renormalize the concentrations of the components according to Eq. (19):

$$m_1' = m_1/(m_1 + m_2) = 0.6/(0.6 + 0.1) = 0.857,$$

$$m_2' = m_2/(m_2 + m_3) = 0.1/(0.1 + 0.3) = 0.250,$$

$$m_3' = m_3/(m_3 + m_1) = 0.3/(0.3 + 0.6) = 0.333.$$

Then

$$\langle \Lambda_{3-1} \rangle = \Lambda_2 m_2' = \Lambda_3 (1 - m_2') = 10\cdot 0.25 + 1000(1 - 0.25) = 752.5,$$

$$\langle \Lambda_{3-2} \rangle = \Lambda_3 m_3' + \Lambda_1 (1 - m_3') = 1000\cdot 0.333 + 1(1 - 0.333) = 333.7,$$

$$\langle \Lambda_{3-3} \rangle = \Lambda_1 m_1' + \Lambda_2 (1 - m_2') = 1\cdot 0.857 + 10(1 - 0.857) = 2.3.$$

In the second stage we find Λ_1', since the first component is uniformly distributed in the "effective" medium consisting of the second and third components in the form of closed disseminations; we use the formula for calculating the thermal conductivity for closed disseminations [1]:

$$\Lambda_1' = \langle \Lambda_{3-1} \rangle \left[1 - \frac{m_1}{\left(1 - \frac{\Lambda_1}{\langle \Lambda_{3-1} \rangle}\right)^{-1} - \frac{1 - m_1}{3}} \right] = 232.3.$$

The structure which forms the second component and the surrounding medium can be described by a model with interpenetrating components [1]. The thermal conductivity of such a struc-

TABLE 2. Thermal Conductivity of Three-Component Mixtures of Various Structures

m_1	m_3	Model 1	Model 2	Model 3	Model 4	Model 5
1	2	3	4	5	6	7
0,1	0,8	801,0	31,6	516,9	729,4	69,9
0,2	0,7	701,2	19,2	417,3	610,9	35,4
0,3	0,6	601,3	14,7	335,4	502,2	22,4
0,4	0,5	501,4	12,4	260,4	402,2	16,1
0,5	0,4	401,5	11,0	195,3	310,0	12,2
0,6	0,3	301,6	9,9	140,5	224,5	9,6
0,7	0,2	201,7	8,7	89,4	145,1	7,2
0,8	0,1	101,8	6,8	40,9	71,3	4,9

ture is given by the formula

$$\Lambda_1' = \langle \Lambda_{3-2} \rangle [c^2 + (1-c)^2\nu + 2\nu c(1-c)/(\nu c + 1 - c)],$$

where the parameter c is found from the graph of Fig. 1 which was taken from [1]: c = 0.804, $\nu = \Lambda_2/\langle\Lambda_{3-2}\rangle = 0.03$. Then

$$\Lambda_2' = 333.7[0.804^2+(1-0.804)^2\cdot 0,03+2\cdot 0.03\cdot 0.804\ (1-0.804)/(0.03\cdot 0.804 + 1 - 0.804)] = 230.4.$$

The third component with the surrounding medium also forms a structure with interpenetrating components, and therefore $c_3 = 0.637$, $\nu_3 = 1000/2.3 = 434.8$,

$$\Lambda_3' = 2.3\,[0.637^2+(1-0.637)^2\cdot 434,8+2\cdot 434,8\cdot 0,637(1-0.637)/(434,8\cdot 0,637 + 1 - 0,637)] = 134.4.$$

From Eq. (17) the effective thermal conductivity of the whole system is

$$\Lambda = 1\,\frac{232.3-752.5}{1-752.5} + 10\,\frac{230.4-333.7}{10-333.7} + 1000\,\frac{134,4-2,3}{1000-2.3} = 137.0.$$

Using this method we calculated the thermal and electrical conductivities of 64 different multicomponent mixtures. The distribution of the differences between the experimental and calculated values obeyed the normal distribution law with a mean-square deviation S = 5%.

We performed special investigations to justify the choice of the layered-structure model to determine the thermal conductivity of the "effective" medium surrounding an element. The medium was modeled by the following structures: 1) layered with layers parallel to the heat flux; 2) layered with layers perpendicular to the heat flux; 3) with interpenetrating components; 4) with isolated disseminations having a thermal conductivity lower than that of the surrounding medium; 5) with isolated disseminations having a thermal conductivity higher than that of the surrounding medium. In the second stage the two-component structure was modeled by a structure with interpenetrating components. Table 1 lists the calculated values of the thermal conductivity of a three-component system with the following values of the thermal conductivity of the components: $\Lambda_1 = 1$, $\Lambda_2 = 10$, $\Lambda_3 = 1000$; the volume concentration of the second component $m_2 = 0.1$, and m_1 and m_3 are varied from 0 to 1.

As can be seen from Table 1, the calculated values of Λ found by using models 1-5 do not differ from one another by more than 10%. From this follow recommendations on the choice of model for calculating thermal conductivities in the first stage. Since the calculated results are practically independent of the model type, the simplest structure is chosen, with n components distributed parallel to the heat flux. In the second stage of the calculation the effect of the structure increases sharply. As an example we recalculate the thermal conductivity of the same three-component mixture, but instead of modeling the system by a structure with interpenetrating components as we did in the preceding case, we now model it with layered structures and structures with isolated disseminations. Table 2 lists the values of the conductivity of the three-component mixture, where each row corresponds to some combination of volume concentrations, and each column to a specific structure. Thus, column 3 corresponds to a layered structure with layers arranged parallel to the direction of the heat flux (in the second stage of the calculation). In the first stage of the calculation a layered structure was taken with layers parallel to the heat flux. Column 4 corresponds to a layered structure with layers perpendicular to the heat flux, column 5 to a structure with interpenetrating components, 6 to a structure with isolated disseminations having a thermal conductivity lower than that of the surrounding medium, and 7 to a structure with isolated disseminations having a thermal conductivity higher than that of the matrix.

Table 2 shows that the values of the thermal conductivity of a mixture calculated with various models may differ by as much as a factor of 40 (e.g., the row with volume concentrations $m_1 = 0.5$, $m_2 = 0.1$, and $m_3 = 0.4$, where $\Lambda_{(1)} = 401.5$, and $\Lambda_{(2)} = 11.0$).

Thus, to increase the accuracy of the calculation it is necessary to know the structure of the mixture, and to take account of it in the second stage of the calculation.

NOTATION

Λ, conductivity of heterogeneous system; $\langle\vec{j}\rangle$, average heat flux; $\langle\vec{\nabla\varphi}\rangle$, average temperature gradient; V, volume of body; Λ_i, conductivity of i-th component; m_i, volume concentration of i-th component; $\vec{j}_i$, flux in i-th component; $\vec{\nabla\varphi_i}$, temperature gradient in i-th component; Ψ_i, ratio of i-th gradient to average; Λ_i', conductivity of system if i-th component is taken as basis; $\langle\Lambda_{n-i}\rangle$, conductivity of n − i components; c, geometric parameter of interpenetrating structure.

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