MATHEMATICAL SIMULATION OF HETEROGENEOUS ISOTROPIC SYSTEMS

G. N. Dul'nev, V. K. Kruglikov,
and E. V. Sakhova

UDC 526.2

The conductivity of multicomponent isotropic heterogeneous system is studied with the help of a computer using statistical analysis.

We will investigate an isotropic heterogeneous system consisting of different polyhedrons, whose components fill the entire space without voids and have different transfer coefficients Λ_i. If i = 2, then a binary system is being examined, while for i > 2, a multicomponent heterogeneous system is being examined. In order to study the transfer coefficients of such materials, in recent years, computer-aided statistical techniques are widely used, which has permitted obtaining important characteristics, unified by the term theory of percolation or percolation processes. The general topological picture of the structure of a binary heterogeneous system as a function of the concentration of components has become clear from the work in [1-3]. Figure 1 represents a binary mixture of polyhedrons, where the dark regions have high conductivity, while the white regions are perfect insulators. Assume that initially the entire space is filled by insulators (Fig. 1a) and, then, a conductor is randomly disseminated into the system. A mathematical experiment on a computer, carried out using the Monte Carlo method, showed that for low concentration m_M (M indicates a metal) of the conducting component, regions with high conductivity appear singly or as small clusters (Fig. 1b). As the system grows, large clusters can form as well, which together with the small clusters form so-called isolated clusters (IsC). When the concentration m_M approaches a critical value m_c ($m_M \to m_c$), the large clusters begin to coalesce with one another and giant clusters with odd shapes appear (Fig. 1c and f), separated from one another by a low nonconducting space A–A. For $m = m_c$, the isolated clusters coalesce and form infinite clusters (InC); the system becomes conducting. With further growth, $m_M > m_c$, the infinite cluster increases, absorbing small clusters, and conducting chains permeate the entire system, forming a system with interpenetrating components (Fig. 1d), and the latter, with $m_M = 1$, becomes a homogeneous (metallic) system (Fig. 1e). The value $m = m_c$ is called the percolation threshold, at which, in a conductor-ideal insulator system, conductivity by "hops" increases from zero to some magnitude and then varies monotonically with increasing concentration m_M. This phenomenon is called hopping conductivity and the existence of a percolation threshold is a general phenomenon inherent both to disordered and lattice models. The effective conductivity Λ of a two-component highly inhomogeneous system $\nu = \Lambda_I/\Lambda_M = 0$, consisting of a mixture of ideal insulators and conductors with conductivities Λ_I and Λ_M, can be described with the help of the following computer-fitted equations [3, 4]:

$$m_c < m \leqslant 0{,}5, \ \Lambda/\Lambda_M = A(m_M - m_c)^K,$$
$$m < m_c, \ \Lambda/\Lambda_I = 1/(1 - 5m_M),$$
$$m_c = 0{,}15 \pm 0{,}03, \ K = 1.8 \pm 0{,}2, \ A = 1\text{—}1.6.$$

In what follows, the conductivity of inhomogeneous systems was investigated with methods in which a computer statistical analysis was combined with different model representations. These methods are reviewed in [5, 6]. In particular, a model constructed based on a combination of the percolation method and reduction to an elementary cell is constructed in [6]. The equations obtained permit finding with satisfactory accuracy the conductivity of isotropic binary systems for any ratio of the conductivities of the components $0 \le \Lambda_1/\Lambda_2 \le 1$ in the entire range of variation of their concentrations $0 \le m_1 = 1 - m_2 \le 1$.

The formation of an infinite cluster and the appearance of hopping conductivity have been studied quite well using statistical methods with the help of a computer for binary media. An important problem is the extension of this problem using the same methods to multicomponent (two and more components) heterogeneous

Institute of Precision Mechanics and Optics, Leningrad. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 41, No. 5, pp. 859-864, November, 1981. Original article submitted July 16, 1980.

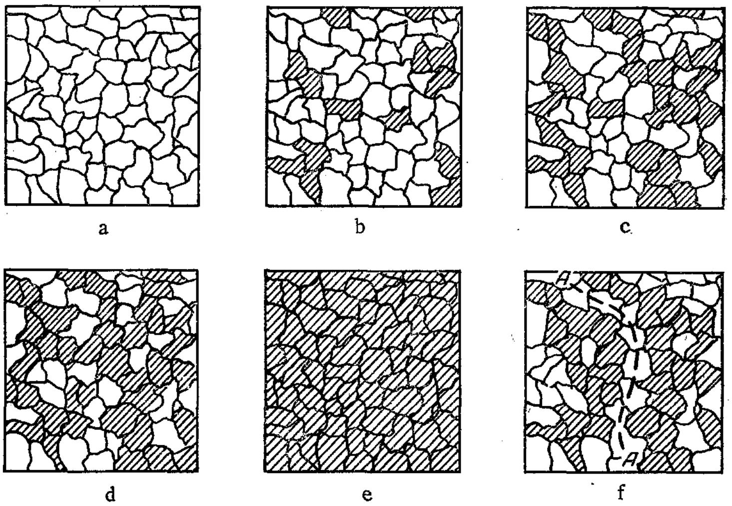

Fig. 1. Model of a binary two-dimensional inhomogeneous body: a) $m_M = 0$; $m_I = 1$; b) $m_I > m_M$, $m_M < m_c$; c and f) isolated clusters; d) $m_M \geq m_c$; e) $m_M = 1$, $m_I = 0$.

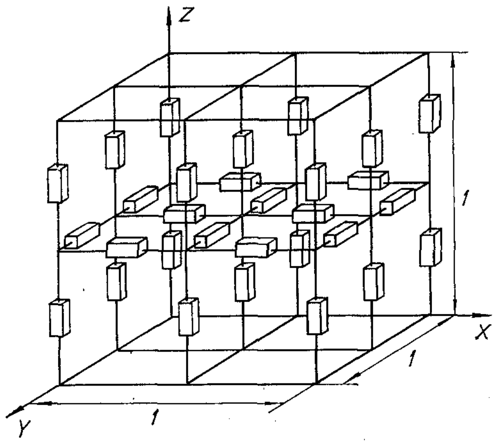

Fig. 2. Model of a heterogeneous system.

systems for arbitrary conductivity of the components.

We point out one more problem, which is most naturally solved by appealing to a mathematical experiment on a computer. In determining experimentally the thermophysical properties of inhomogeneous systems or in calculating their temperature fields, the inhomogeneous system is usually replaced by a quasihomogeneous body with some effective properties. In so doing, it is necessary to estimate the dimensions of the so-called representative element of the system, whose transport coefficient is approximately equal to the transport coefficient of the entire mass. In what follows, we present methods for solving such problems and results of solutions.

We examine first a binary heterogeneous system with a random distribution of components (Fig. 1) and we will choose from the system some cube, in which the concentration of components equals the corresponding concentration in the entire mass; we will assume that the lengths of the cube edges equal unity and that the lateral surfaces of the cube are adiabatic, i.e.,

$$\left.\frac{\partial t}{\partial x}\right|_{x=0} = \left.\frac{\partial t}{\partial x}\right|_{x=1} = 0; \left.\frac{\partial t}{\partial y}\right|_{y=0} = \left.\frac{\partial t}{\partial y}\right|_{y=1} = 0, \tag{1}$$

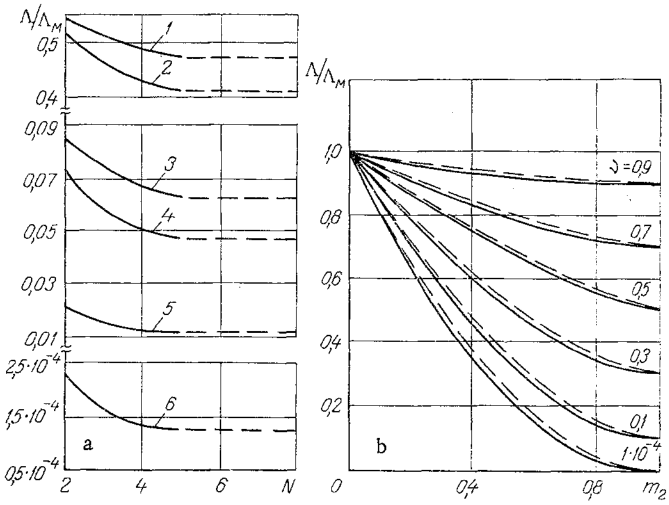

Fig. 3. Dependence of the conductivity of a binary heterogeneous system on the number of layers in the model (a) [1) $\Lambda/\Lambda_M = 1 \cdot 10^{-2}$, $m_2 = 0.3$; 2) $1 \cdot 10^{-4}$ and 0.3; 3) $1 \cdot 10^{-2}$ and 0.7; 4) $1 \cdot 10^{-4}$ and 0.7; 5) $1 \cdot 10^{-2}$ and 0.9; 6) $1 \cdot 10^{-4}$ and 0.9] and on concentration (b).

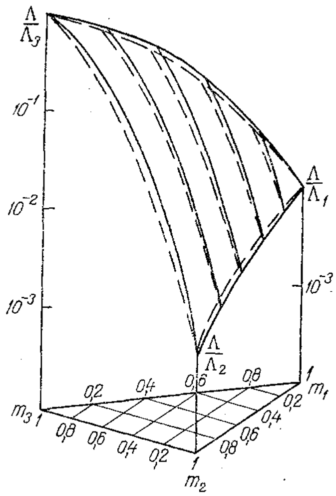

Fig. 4. Concentration dependence of the conductivity of a three-component system.

while the surfaces z = 0 and z = 1 are isothermal (Fig. 2)

$$t|_{z=0} = t', \quad t|_{z=1} = t''. \tag{2}$$

The basic method for studying the conductivity through such a system is to simulate the system with the help of a collection of connected resistances. We separate the cube being examined by planes parallel to the base into N layers and each layer in its turn into N^2 parts with planes parallel to the lateral faces. Resistances of some type are positioned between the nodes of the lattice obtained and the number of each type of resistance is proportional to the concentration of the components (Fig. 2). With the help of a pseudorandom number generator, the magnitude of the resistances is assigned one of two possible values. We will denote the conductivities of the components by Λ_1 and Λ_2, and their concentrations by m_1 and m_2 ($m_1 + m_2 = 1$), and we will find the overall resistance R to a flow Q between the isothermal surfaces:

$$R=\frac{t''-t'}{Q}. \tag{3}$$

For a single cube, the area of the isothermal surface and the height of the cube equal unity, so that the effective conductivity is $\Lambda = R^{-1}$. If we assume that $t' = 0$ and $t'' = 1$, then we obtain from (3) $\Lambda = Q$, i.e., the problem reduces to determining the flux passing through the cube. We first find the magnitude of the flux Q_1 flowing through the first layer, in which there are M^2 resistances, while $M = N + 1$. We denote by $i = 1, 2, \ldots, M^2$ the numbers ordering the nodes; $\Lambda_{i,\,i+M^2}$, conductivity between neighboring nodes along the OZ axis; S_i, area per resistance; and $\delta = 1/N$, thickness of a single layer. The magnitude of the flux Q_1 is given by

$$Q_1=\frac{1}{\delta}\sum_{i=1}^{M^2}\Lambda_{i,i+M^2}(t_{i+M^2}-t_i)\,S_i, \tag{4}$$

where t_{i+M^2} and t_i are the temperatures at neighboring points along the OZ axis.

In order to determine the temperature field of the model, we will write the equation for balance of heat energy at the i-th point:

$$\begin{gathered}(\Lambda_{i,i+1}+\Lambda_{i,i-1}+\Lambda_{i,i+M}+\Lambda_{i,i-M}+\Lambda_{i,i+M^2}+\\ +\Lambda_{i,i-M^2})\,t_i-\Lambda_{i-1,i}t_{i-1}-\Lambda_{i+1,i}t_{i+1}-\Lambda_{i-M,i}\,t_{i-M}-\Lambda_{i+M,i}\,t_{i+M}-\Lambda_{i-M^2,i}t_{i-M^2}-\Lambda_{i+M^2,i}t_{i+M^2}=0,\end{gathered} \tag{5}$$

where $\Lambda_{i,i-1}$; $\Lambda_{i,i+1}$ are the conductivity between neighboring points along the OY axis; $\Lambda_{i,i-M^2}$; $\Lambda_{i,i+M^2}$ are the conductivity between neighboring points along the OZ axis; $\Lambda_{i,i-M}$; $\Lambda_{i,i+M}$ are the conductivity between neighboring points along the OX axis. Equation (5) can be written in a different form as follows:

$$t_i\sum_{j=M^2+1}^{M^3-M^2}\Lambda_{ij}-\sum_{j=M^2+1}^{M^3-M^2}t_j\Lambda_{ij}=0,$$

and, in addition,

$$\Lambda_{ij}\neq 0 \ \text{for} \ \begin{cases} j=i-1;\ i+1,\\ j=i-M;\ i+M,\\ j=i-M^2;\ i+M^2.\end{cases} \tag{6}$$

If Eq. (6) is written for all values of $i = M^2 + 1, M^2 + 2, \ldots, M^3 - M^2$, then we obtain a system of ordinary algebraic equations, whose solution determines the temperature field of the model. According to the conditions of the problem, for a stationary process, the flux passing through a single layer equals the flux passing through the entire cube. The system of equations (4) and (6) was solved using the Monte Carlo technique on an ES-1022 computer. Using the method indicated, we determined the dimensions of a representative element of a binary heterogeneous system. For this, we calculated the effective conductivity of the Λ model, containing from two to five layers. Figure 3a shows the dependence of $\Lambda = f(N, \nu)$ conductivity on the number of layers N for different values of the ratio $\nu = \Lambda_2/\Lambda_1$. From the results obtained, we can draw the following conclusions:

a) the value of Λ_2/Λ_1 has practically no effect on the choice of the representative element;

b) the deviation of Λ from the limiting value (Λ_∞ for $N \to \infty$) increases with increasing concentration of the nonconducting component;

c) over the entire range of concentrations, the results obtained with the five-layer model do not deviate from the limiting values by more than 5%. Thus, the representative element of a binary heterogeneous system must contain at least five layers.

The conductivity of multicomponent systems was subsequently studied using the five-layer model. Figure 3b shows the results of a calculation of Λ for a binary system with different values of Λ_2/Λ_1 over the entire range of variation of concentrations $0 \le m_2 \le 1$ (continuous lines); the dashed lines in this figure indicate the dependences calculated using the equations obtained by simulation, proposed by Dul'nev and Novikov [5, 6].

The conductivity of a three-component system was investigated using the same model. The values of the resistance of the first, second, and third types were distributed among the nodes of the model in two stages. In the first stage, bonds were chosen for which the values of the resistances corresponding to the first component were assigned in a random manner; the number of such bonds was determined by the volume concentration m_1. At the second stage, the values of the given volume concentration of the remaining two components were renormalized:

$$m_2' = \frac{m_2}{1-m_1}, \; m_3' = \frac{m_3}{1-m_1}, \tag{7}$$

where m_2' and m_3' are the new values of the volume concentration of the second and third components and, in addition, $m_2' + m_1' = 1$. The values of the resistances of the second and third components were distributed according to the values of the concentrations obtained. Figure 4 shows the results of the calculation of the effective conductivity of a three-component system; the dashed lines indicate the values obtained from the model representations based on a self-consistent method [7].

NOTATION

Λ, conductivity of the heterogeneous system; Λ_i, conductivity of the i-th component; m_i, volume concentration of the i-th component; m_M and m_I, volume concentrations of the conducting and nonconducting (insulating) components.

LITERATURE CITED

1. S. Kirkpatrick, "Percolation and conduction," Rev. Mod. Phys., 45, No. 4, 574-588 (1973).
2. B. I. Shklovskii and A. L. Éfros, "Theory of percolation and conduction in strongly inhomogeneous media," Usp. Fiz. Nauk, 117, No. 3, 401-434 (1975).
3. V. K. Shante and S. Kirkpatrick, "An introduction to percolation theory," Adv. Phys. (London), 20, No. 85, 325-357 (1971).
4. I. Webman, J. Jortner, and M. Cohen, "Electronic transport in alkalitungsten bronzes," Phys. Rev. B, 13, No. 2, 713-727 (1976).
5. G. N. Dul'nev, Transport Coefficients in Inhomogeneous Media [in Russian], Leningrad Institute of Precision Mechanics and Optics, Leningrad (1979).
6. G. N. Dul'nev and V. V. Novikov, "Conductivity of inhomogeneous systems," Inzh.-Fiz. Zh., 36, No. 5, 901-910 (1979).
7. G. N. Dul'nev, B. L. Muratova, and V. V. Novikov, "Conductivity of multicomponent heterogeneous systems," Inzh.-Fiz. Zh., 41, No. 4, 593-600 (1981).