## NOTATION

T) temperature; v) growth rate; z) direction of growth; S) crystal surface; n) normal to S; $\rho(x)$) radius of curvature of S; x) radius vector (x, y, z); (r, $\varphi$)) polar coordinates in the x–y plane; D) thermal conductivity; $c_i$, i = 1, 2) heat capacity; L) latent heat of melting; $\varepsilon$) surface internal energy; $\gamma$) surface free energy; $T_{melt}$) melting temperature of a planar crystal; K) linear kinetic coefficient; $l = 2D/v$) length scale; $t = (T - T_\infty)c_2L^{-1}$) nondimensional temperature; $p = v\rho_0/2D$) Peclet number. The subscripts i = 1, 2 denote the solid and liquid phases respectively; primes denote nondimensional quantities.

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# DETERMINING THE THERMAL CONDUCTIVITY OF CERAMIC MATERIALS BY SOLVING THE INVERSE HEAT-CONDUCTION PROBLEM


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A method is propounded for determining the temperature dependence of the thermal conductivity of ceramic materials. It is based on a solution of the inverse heat-conduction problem. An installation is described for carrying out the thermophysical experiment. The temperature dependence of thermal conductivity of a ceramic material has been obtained.


The implementation of effective high-temeprature processes and equipment depends to a large extent on investigations of materials, and a considerable part of this consists of exploring the thermophysical characteristics of the materials. Such investigations, as a rule, reduce to solving a number of complex technical and mathematical problems. This applies to the experimental-computational determination of thermal conductivity, although here it is usually not necessary that a temperature field varying according to a specified program be maintained, it being sufficient to ensure a stable steady-state heat transfer. Nonetheless, growing demands for precision in the determination of thermal conductivity over a wide temperature range make it necessary to perfect both the techniques of the thermal experiment and the processing of the results. Very promising in this connection is the use of methods of solving the inverse heat-conduction problem (IHCP) [1, 2], allowing a widening of the range of variation of thermal loading of the specimen, which is suitable for the indirect measurement of thermal conductivity. This makes it possible to lower the demand for precise experimental data, and to raise the quality of identifying the thermal conductivity, by simultaneous processing of information received from a large number of points at which temperature is monitored, or under the conditions of an increased number of variants of thermal loading. Advantages of the IHCP methods consist of being able to take into account properly and without special difficulties, the dependence of thermophysical properties on


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temperature. This is especially important because the thermophysical properties of most materials depend significantly on temperature. During heating, the thermal conductivity of ceramic materials falls sharply, sometimes by ten times [3]. Neglecting this may lead to inadmissible errors in heat engineering calculations. For taking into account the temperature dependence of thermal conductivity it is necessary to resort to increased complication in the procedure for modeling the temperature fields, using, for this, special methods and computing techniques. Here, as a rule, numerical as opposed to analytic methods are used. This is because of the nonlinearity, especially with multidimensional arrangements, and compl configuration of the objects examined.

In the present work special attention is given to a procedure for modeling nonlinear thermal processes in multilayered objects, which may be ascribed to the numerical-analytic methods for solving the heat-conduction problem.

A determination of the temperature dependence of thermal conductivity $\lambda(T)$ with the aid of the proposed method is implemented in accordance with one of the strategies for solvir the intrinsic IHCP described in detail in [4, 5]. This strategy proposes multiple modeling of the temperature field of the specimen being studied, accompanied by a selection of the parameters of the dependence of thermal conductivity on temperature being sought. The solution will be attained when the averaged divergence between the modeled and experimentally observed temperatures becomes equal to the measuring accuracy or reaches a minimum.

The effectiveness of the solution of the inverse problem and also the expenditure of machine time and memory are determined chiefly by the structure of the modeling procedure. The modeling of a thermal process in a nonlinear medium can be simplified if the original nonlinear heat flow equation is transformed beforehand, as for example with the aid of the Kirchhoff substitution:

$$\Theta = \int_0^T \lambda(T)\,dT. \tag{1}$$

This makes it possible to eliminate the nonlinearity in the left part of the heat-conduction equation, and to make the majority of the coefficients of the corresponding system of finite-difference equations into constants. It is true that the boundary conditions sometimes there by become complicated, and it becomes necessary to introduce in the computing scheme a block performing the inverse transformation of the function $\Theta$ into T. The inverse transform process, with its apparent complexity and ambiguity, has limited considerably the field of use of methods employing the Kirchhoff and Goodman transformations. The additional effort expenditure (incidentally, not so large) associated with the inverse transformation is, however, repaid by the increased speed of computations on a digital computer, or the simplification and decreased cost of computing when the modeling is done on an analog or hybrid computer.

The choice of computing method for making the transformation $T(\Theta)$ is largely determined by its being single-valued, on account of the strict positivity of the function $\lambda(T)$.

Since $\lambda(T)$ is usually the result of an analytic approximation of the dependence in tabular form, it is necessary that the condition $\lambda(T) > 0$ be fulfilled at least in the temperature interval $[T_{min}, T_{max}]$ characteristic of the given heat-conduction problem. Then $\Theta(T)$, as the integral of a positive function, will grow monotonically in this interval, i.e., a reciprocal single-valued correspondence between T and $\Theta$ is always observed in the range $[T_{min}, T_{max}]$.

Thus, the temperature value corresponding to the known $\Theta$ may be found as a root of the equation

$$\Theta(T) - \Theta = 0,$$

and in the interval $[T_{min}, T_{max}]$ there will be only one root. It is convenient to find it by a one-dimensional search for the minimum of the difference function

$$E(T) = |\Theta(T) - \Theta| \quad \text{or} \quad E(T) = (\Theta(T) - \Theta)^2.$$

It is important to note that the transformation may be implemented both for continuous and piecewise continuous dependences $\lambda(T)$. Let, for example, the temperature interval

$[T_{min}, T_{max}]$ be broken into s intervals, with the temperature dependence of thermal conductivity in each of these being represented by different functions:

$$\lambda(T) = \begin{cases} \lambda_1(T), & T_{min} \leqslant T < T_1, \\ \lambda_2(T), & T_1 \leqslant T < T_2, \\ \dots & \dots \\ \lambda_s(T), & T_{s-1} \leqslant T \leqslant T_{max}. \end{cases}$$

In this case the Kirchhoff transformation is written

$$\Theta(T) = \begin{cases} \int\limits_0^T \lambda_1(T)\,dT, & T_{min} \leqslant T < T_1, \\ \int\limits_0^{T_1} \lambda_1(T)\,dT + \int\limits_{T_1}^{T} \lambda_2(T)\,dT, & T_1 \leqslant T < T_2, \\ \dots & \dots \\ \int\limits_0^{T_1} \lambda_1(T)\,dT + \sum\limits_{i=2}^{s-1} \int\limits_{T_{i-1}}^{T_i} \lambda_i(T)\,dT + \int\limits_{T_{s-1}}^{T} \lambda_s(T), & T_{s-1} \leqslant T \leqslant T_{max}. \end{cases}$$

This function has the properties of continuity and monotonicity. Hence, even in the case in which the thermal conductivity is represented by piecewise continuous functions, it is possible to use the Kirchhoff substitution. In particular, the use of this substitution proves to be effective when $\lambda(T)$ is given in the form of polynomial splines, including the piecewise-constant, piecewise-linear, and piecewise-quadratic functions often used in heat engineering calculations.

The methods described above are suitable not only for homogeneous media, but also in calculations of the thermal state of heterogeneous systems. These methods allow the volume of computing to be reduced in many important practical cases. For example, the solution of IHCP, the aim of which is the identification of thermophysical characteristics, often reduces to multiple modeling of the temperature field of an object consisting of a layer of the material being investigated and one or more layers of standard materials. At each stage of the modeling, a nonlinear heat-conduction problem is solved, each time with a new variant of the temperature dependences of thermophysical properties. If this inverse problem will be solved by a net method, without prior linearization of the heat-conduction equation, then at each stage of the modeling, the error in the solution will be increased owing to systematic error of the finite-difference approximation, the more so the larger are the differences in the thermophysical properties of neighboring layers, and the more pronounced their dependence on temperature. The Kirchhoff substitution mitigates this problem, and in the solution of the steady-state one-dimensional problem reduces systematic error practically to zero. This is illustrated by the following example of a solution of the heat-conduction problem for a multilayered plate.

Let us suppose that the temperatures $T_{min}$ and $T_{max}$ on the surfaces of the plate are known, i.e., boundary conditions of the 1st kind are specified. Information about the thermal conductivities of all s layers is available in the form of a piecewise continuous functions $\lambda_1(T)$, $\lambda_2(T)$, ..., $\lambda_s(T)$. Also known are the temperature dependences of the thermal contact resistances between layers $R_{C_1}(T)$, $R_{C_2}(T)$, ..., $R_{C_{s-1}}(T)$.

For linearizing the heat-conduction equations in each layer, we make the substitution

$$\Theta_i(T) = \int\limits_0^T \lambda_i(T) + C_i, \quad i = 1, s.$$

Here, in distinction to Eq. (1), there is an unknown coefficient $C_i$ which is needed for matching the functions $\Theta_i$ at the junctions of the layers.

We stipulate continuity of the function $\Theta(x)$ throughout the whole region of the problem [0, L]. It is guaranteed inside the layers by the properties of function $\Theta_i$, and, with x corresponding to the boundaries of the layers $l_1$, $l_2$, ..., $l_{s-1}$, by the condition

$$\Theta_i(l_i) = \Theta_{i+1}(l_i), \quad i = \overline{1, s-1}. \tag{2}$$

Since at the boundaries of the layers the function T(x) is discontinuous on account of the thermal resistance, one and the same coordinate will correspond to two temperatures. These are the maximum $T_{max_i}$ of one layer and the minimum $T_{min_{i+1}}$ of the neighboring layer. Following from this, Eq. (2) may be written in the form

$$\Theta_i(T_{max_i}) = \Theta_{i+1}(T_{min_{i+1}}), \quad i = \overline{1,\ s-1}.$$

From this we get formulas for calculating the unknown coefficients

$$C_{i+1} = \int_0^{T_{min_{i+1}}} \lambda_{i+1}(T)\,dT - \int_0^{T_{max_i}} \lambda_i(T)\,dT + C_i, \quad i = \overline{1,\ s-1}. \tag{3}$$

The coefficient $C_1$ may be fixed arbitrarily, for example, $C_1 = 0$.

The relationship between $T_{min_{i+1}}$ and $T_{max_i}$ is determined by the boundary conditions of the 4th sort. Having chosen at the first stage of the solution of the problem the temperatures $T_{min_2}$, $T_{min_3}$, ..., $T_{min_s}$ as unknowns, we represent the maximum temperatures of the surfaces of the contacts in the form

$$T_{max_i} = T_{min_{i+1}} - R_{Ci}\left(\frac{T_{max_i} + T_{min_{i+1}}}{2}\right) q, \quad i = \overline{1,\ s-1}, \tag{4}$$

where q is the heat flux density, $q = [\Theta_s(T_{max}) - \Theta_1(T_{min})]/L$.

The conditions for the conjugation of layers, determining the equalities of flows, and expression (2) lead to the known solution of the one-dimensional steady-state linear heat-conduction problem, when $\Theta(x)$ is a continuous linear function. Therefore, the system of equations in terms of $T_{min}$ may be written in the following way:

$$\Theta_i(T_{min_i}) = \Theta_1(T_{min}) + l_{i-1}q, \quad i = \overline{2,\ s}. \tag{5}$$

This system of nonlinear algebraic equations can be solved by iterative methods, as, for example, by numerical minimization of the sum of the squares of the relative difference between the right and left parts of the system:

$$E = \sum_{i=2}^{s} [\Theta_i(T_{min_i})/(\Theta_1(T_{min}) + l_{i-1}q) - 1]^2.$$

At the second stage of the solution, having determined $T_{min_i}$, $T_{max_i}$, and $C_i$, we can calculate

$$\Theta(x) = \Theta_i(T_{min_i}) + \frac{x - l_{i-1}}{l_i - l_{i-1}}(\Theta_i(T_{max_i}) - \Theta_i(T_{min_i})), \quad l_{i-1} \leqslant x < l_i,$$

and then, using the inverse Kirchhoff transform procedure, obtain T(x).

As a whole, the iteration process of calculating T(x) is organized in the following way: after the choice of the initial approximation $T_{min_i}^{(0)}$, for example, as

$$T_{min_i}^{(0)} = T_{min} + l_{i-1}(T_{max} - T_{min})/L, \quad i = \overline{2,\ s},$$

$C_i^{(0)}$ is calculated from Eqs. (3) and (4). The difference from the system of Eq. (5) is determined, and, by one of the minimum-seeking strategies, the desired degree of approximation of this difference to zero is attained. Knowing the coordinate values of the minimum, the quantities $\Theta(x)$ and then T(x) can be obtained at the given points.

The approach described makes it possible to solve the forward nonlinear steady-state heat-conduction problem without a large expenditure of machine time. Solution of the problem with similar accuracy by finite-difference methods takes ten times longer. Using the described procedure for modeling the heat-transfer process in a two-layer object allows the intrinsic problem of the temperature dependence of thermal conductivity of composition ceramic materials to be solved efficiently.

A thermophysical experiment with the test materials was carried out in a unit specially constructed for this purpose, a diagram of which is given in Fig. 1. In the unit are the

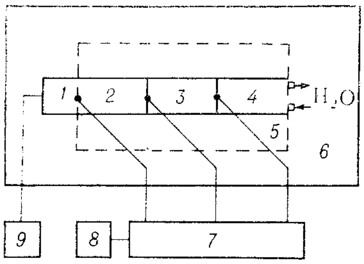


Fig. 1

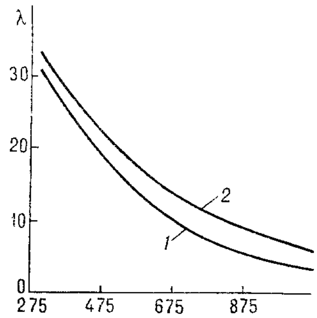


Fig. 2

Fig. 1. Block diagram of the unit used for carrying out the experiment.

Fig. 2. Comparison of the dependence of λ(W/m·K) on T(K), as the result of solving the control problem (1), and with known thermal conductivity $Al_2O_3$ (2).

following blocks: 1) heater; 2) specimen of material of known thermal conductivity; 3) specimen of material of unknown thermal conductivity; 4) refrigerator; 5) heat-reflecting screen; 6) vacuum chamber; 7) commutator; 8) device for recording thermometric information; and 9) block for setting the temperature regime. The installation was based on the VUP-5 universal vacuum station.

The heater is a hollow metal cylinder, inside which is housed a tungsten spiral. Control of the heater is by means of block 9, which allows the temperature to be set with discretization ±0.1 K, and also permits the heater temperature to be changed over a wide range when using a nonstationary regime for measuring thermal conductivity.

The reference and test specimens were made in the form of cylinders of diameter 10 mm and length 30 mm. The refrigerator consisted of a hollow copper cylinder with internal water cooling.

The heat-reflecting cylindrical screen, constructed of metal foil, was intended to reduce the radial component of lateral heat leaks. A reliable barrier for the convective component of these leaks was evacuation to a pressure of $1.3 \times 10^{-4}$ Pa. A directed heat flow is thus created, and the reference–test specimen system can be considered as a two-layer flat semi-infinite plate. Thermometric information is taken off by the recording arrangement, which is switched in turn via a commutator to three temperature sensors.

This experimental unit allows the test material to be heated to 1300 K, and the temperature can be recorded at three points in the reference–test specimen system, which makes it possible to solve the IHCP to get reliable information on the temperature dependence of thermal conductivity through the temperature range important in practice.

An evaluation of the accuracy of the determination of thermal conductivity was made by solving a control problem, the results of which are given in Fig. 2.

Aluminum oxide was used as a test material, the thermal conductivity data of which are given in [6]. The upper curve of Fig. 2 was drawn from this source, and the lower curve from the results obtained by solving the IHCP. With agreement in the general character of the curves, a difference, reaching 20-30%, is seen in the values of thermal conductivity. This may have been caused not only by experimental and computing errors, but also by the presence of impurities, preculiarities of the technology of preparing specimens, etc.

Following the method described for solving the IHCP, we obtained the temperature dependence of thermal conductivity of a new promising thermoinsulating material, in the composition of which aluminum oxide was dominant. This dependence in the temperature range from 275 to 875 K was found in the form of a single analytic function, consisting of a linear combination of high-order Chebyshev polynomials. As input information we took temperature data obtained from the test specimen and copper standard in 20 experiments over different temperature ranges in the experimental unit described above.

The function λ(T) is shown graphically in Fig. 3. At temperatures above 675 K (Fig. 3b) the thermal conductivity falls to a value typical of highly effective thermal insulators.

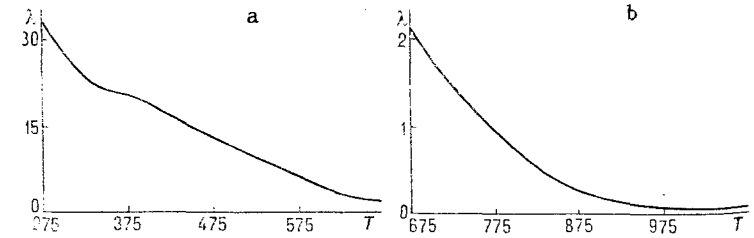


Fig. 3. Dependence of λ on T for the material studied in the two temperature ranges, K: a) 275-675; b) 675-875.

It is, moreover, lower than that of pure aluminum oxide. This is explained by the presence in the test material, apart from aluminum oxide, of other specially chosen components which also give it the necessary durability and guarantee high production effectiveness in the manufacture of various heat-reflecting components and coatings.

## NOTATION

$\lambda(T)$, temperature dependence of thermal conductivity; $\Theta$, quantity introduced by Kirchhoff substitution; $T_{min}$, $T_{max}$, bounds of the temperature range; E, difference value; s, number of intervals; $R_C$, thermal contact resistance; C, undefined constant; x, spatial coordinate; L, length; q, heat flux density.

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# CALCULATION OF THE DIFFUSION COEFFICIENTS OF ALKALI AND ALKALI-EARTH METAL VAPOR IN HELIUM BY EXCHANGE PERTURBATION ANALYSIS

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The potential energy of metal–helium interaction is calculated by the quantum-mechanical exchange perturbation theory. The results are used to calculate the diffusion coefficient of alkali and alkali-earth metal vapor in helium. The values of the saturated-vapor pressure of barium at 1170-1420 K are refined from a comparison with experimental diffusion data.

Calculation of the diffusion coefficient of monoatomic vapor of metals in helium from the formula of the first-approximation Enskog–Chapman theory [1]

$$PD_{12} = \frac{3}{16\pi} \frac{\sqrt{2\pi (kT)^3/m_{12}}}{\sigma_{12}^2 \Omega_{12}^{(1,1)*}} \tag{1}$$

requires that the potential energy $\varphi(R)$ of the interatomic interaction be known. The reduced collision integral $\Omega_{12}^{(1,1)*}$ and the cross section $Q_{12}^{(1,1)} \equiv \sigma_{12}^2 \Omega^{(1,1)*}$ depend on this energy.

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