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APPLICATION OF NUMERICAL METHODS TO SOLVE NONLINEAR INVERSE PROBLEMS IN CALORIMETRY OF HARD MATERIALS

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A method is suggested for numerical determination of heat capacity as a function of temperature using the data on nonstationary experiments. This is based on the solution of the inverse problem in the overdefined formulation, with allowance for the temperature distribution inside the solid. The algorithm developed for the solution of the problem allows determination of the heat capacity both in case of a material with a known thermal conductivity, and in the case when the thermal conductivity of the material is unknown and should be determined simultaneously with the heat capacity. The suggested method of numerical solution for the coefficient-type inverse problem of nonlinear thermal conductivity may also be of use in interpretations of the data of thermal analysis.

In determining the heat capacities of hard materials by nonstationary methods, which are widely employed due to the convenience of applying a computer (in contrast to stationary methods), one is confronted with the problem of a nonuniform temperature distribution in a solid; this cannot be taken into account correctly by analytical means in the general case. Different methods of introducing "basic" and "mean volume" temperature as references for the measurement results [1] are not theoretically validated, and their successful application depends to a large extent on the experience and intuition of the experimenter. This question can be clarified if the inverse problem is solved in the extremal formulation by means of numerical methods [2, 3].

The present paper suggests a method for numerical identification of the heat capacity as a function of temperature; it is based on the solution of the inverse problem in the overdefined formulation, with allowance for the temperature distribution inside the solid. The algorithm developed for the solution of this problem can be used both in the case of a material with known thermal conductivity and in the case when the thermal conductivity of the material is unknown and should be determined simultaneously with the heat capacity. The suggested method of numerical solution for the coefficient-type inverse problem of nonlinear thermal conductivity may also be of use in interpretations of the data of thermal analysis.

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To determine the volumetric heat capacity for specimens of canonical shape (a plate for $n = 0$, or a cylinder for $n = 1$), the following formulation of the problem is used with the known boundary conditions:

$$\vartheta(0, t) = \vartheta_1 (t), \quad \vartheta(1,t) = \vartheta_2 (t) \tag{1}$$

$$\frac{\partial \vartheta}{\partial x} (0,t) = 0, \quad \lambda \frac{\partial \vartheta}{\partial x} (1,t) = -\sigma (t) \tag{2}$$

for the equation of thermal conductivity:

$$C(\vartheta) \frac{\partial \vartheta}{\partial t} = x^{-n} \frac{\partial}{\partial x} x^n \lambda(\vartheta) \frac{\partial \vartheta}{\partial x} \tag{3}$$

with the initial condition:

$$\vartheta(x,0) = \vartheta_o (x) \equiv 0 \tag{4}$$

to find the heat capacity satisfying the inequality:

$$C(\vartheta) > 0 \tag{5}$$

If $\lambda(\vartheta)$ is also to be determined, then a condition similar to (5) is at least known for it:

$$\lambda(\vartheta) > 0 \tag{6}$$

In Eqs (1–3) all the values are considered to be appropriately dimensionless (normalized): ϑ is the dimensionless temperature, x is the coordinate, t is the time, λ is the thermal conductivity, C is the heat capacity (dimensional volumetric heat capacity $= C_{\text{dim}} = c\rho$, where c is the specific heat capacity and ρ is the density), and σ is the specific heat flux into the specimen.

The function $C(\vartheta)$ is found by the successive interval method (Fig. 1) in the parameter form:

$$C^k (\vartheta) = g \left(\sum_{i=1}^{n_c} C_i^k (\vartheta - \vartheta^k)^{i-1}\right) \tag{7}$$

Having determined the parameters of C_i^k for the k-th interval, we proceed to the $(k + 1)$-th interval. In Eq. (7), ϑ^k is the temperature corresponding to the beginning of the k-th time interval (see Fig. 1), and $g(S)$ is the functional conversion providing an account of a priori conditions for $C(\vartheta)$. In particular, the positive condition (5) is taken into account by the choice $g(S)$ exp (S). If $\lambda(\vartheta)$ is to be determined in addition to $C(\vartheta)$, it is also represented as

$$\lambda^k(\vartheta) = g\left(\sum_{i=1}^{n_\lambda} \lambda_i^k (\vartheta - \vartheta^k)^{i-1}\right) \tag{8}$$

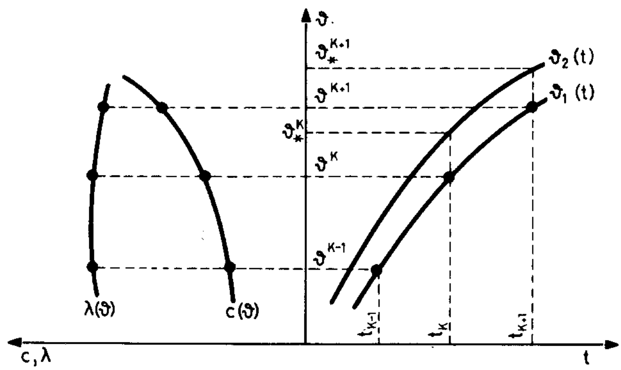

Fig. 1 Successive interval parameterization of desired dependences.

Proceeding to the extremal formulation of the inverse problem, we shall find the parameters C_i^k from the condition of the minimum for caloric mismatch:

$$Y[C^k(\vartheta)] = \frac{1}{2} \int_{t_k}^{t_{k+1}} \left[\int_o^1 x^n C^k \frac{\partial \vartheta}{\partial t} \, dx - \sigma(t) \right]^2 dt \to \inf C_i^k \tag{9}$$

The minimized functional is obtained from the balance equation for the total amount of heat. In calculations of the values Y as $\vartheta(x,t)$, the solution of the first boundary-value problem (3), (1) with the initial condition obtained for the previous, $(k-1)$-th interval is taken:

$$\vartheta_o(x) = \vartheta(x, t_k; C^{k-1}) \tag{10}$$

The appropriate method of minimization is the method of conjugate gradients [2], in which it is necessary to know the values of gradients at the points of minimizing sequence. To calculate the gradient components, we shall apply the conjugate problem method [4]. According to this method:

$$\frac{\partial Y}{\partial C_i^k} = \int_{t_k}^{t_{k+1}} \int_o^1 x^n \varphi \frac{\partial \vartheta}{\partial t} \frac{\partial c}{\partial c_i^k} \, dx \, dt \qquad (11)$$

where φ is the solution of the boundary-value problem conjugated to Eq. (9):

$$x^n \frac{\partial \varphi}{\partial \tau} = a^k \frac{\partial}{\partial x} x^n \frac{\partial \varphi}{\partial x},$$

$$\varphi(x,0) = 0; \; \varphi(0,\tau) = 0, \quad \varphi(1,\tau) = B(t_{k+1} - \tau) \qquad (12)$$

In Eqs (12), $\tau = t_{k+1} - t$ is an inverse time, $B(t)$ is the caloric mismatch contained in brackets in Eq. (9), and $a^k = \lambda / C^k$ is the thermal diffusivity.

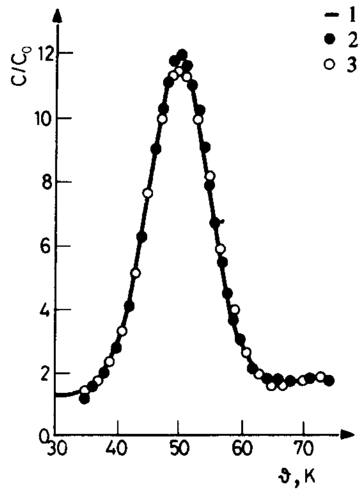

Fig. 2 Determination of heat capacity for a cylindrical specimen ($n = 1$): 1 – exact values, 2 – reconstructed heat capacity for exactly known thermal conductivity $\lambda = \lambda_o \cdot (1+5 \cdot 10^{-4}\ \vartheta)$, 3 – reconstructed heat capacity for incorrect thermal conductivity $\lambda = 1.1\ \lambda_o$.

Figure 2 shows the results of solving the methodical problem on $C(\vartheta)$ reconstruction by means of a computer. The form of $C(\vartheta)$ was set similar to that usually used for the effective heat capacity on the melting, for example, of mixtures of paraffins. It is seen that, even if the thermal conductivity is known only with appreciable error, the heat capacity of essentially nonlinear form is determined reasonably well (error near maximum ~5-6%, in sections adjoining the peak region ~2-3%). In the numerical solution of the inverse problem with the stated algorithm, the logarithm of the effective volumetric heat capacity at intervals was approximated by a cubic parabola ($n_c = 4$), with joining carried out with the value of the heat capacity (this decreases the number of desired parameters by one) at the end of the intervals. The value of the temperature-time interval was chosen from the condition:

$$\vartheta^{k+1} - \vartheta^k = \alpha = \text{const}$$

The algorithm for the simultaneous determination of $C(\vartheta)$ and $\lambda(\vartheta)$, if the latter is unknown, is based on a weak sensitivity of functional Y to the values of the thermal conductivity (with an error in the thermal conductivity up to 50%, the heat capacity is determined from Eq. (9) with an error of not more than ~10-12%). The thermal conductivity represented by parameters in accordance with Eq. (8) found from the functional minimization:

$$Z[\lambda^k(\vartheta)] = \frac{1}{2} \int_{t_k}^{t_{k+1}} [\int_o^1 \frac{x^{-n} q}{\lambda^k} \, dx - (\vartheta_1 - \vartheta_2)]^2 \, dt \rightarrow \inf \lambda_i^k \qquad (13)$$

In Eq. (13), $q(x,t) = -x^n \lambda \frac{\partial \vartheta}{\partial x}$ is the dimensionless specific heat flux in the solid; simultaneously with the temperature field, this is found from the solution of the second boundary-value problem for a set of equations:

$$x^n c^k \frac{\partial \vartheta}{\partial t} + \frac{\partial q}{\partial x} = 0, \quad x^n \lambda^k \frac{\partial \vartheta}{\partial x} + q = 0 \qquad (14)$$

with boundary conditions (2) and the initial condition:

$$\vartheta_o(x) = \vartheta(x, t_k; C^{k-1}, \lambda^{k-1}) \qquad (15)$$

The values of the components for the functional gradient are calculated by the conjugate problem method using the equations:

$$\frac{\partial Z}{\partial \lambda_i^k} = \int_{t_k}^{t_{k+1}} \int_o^1 \Psi \frac{\partial \vartheta}{\partial x} \frac{\partial \lambda}{\partial \lambda_i^k} \, dx \, dt \qquad (16)$$

$$x^n \frac{\partial \varphi}{\partial \tau} - a^k \frac{\partial \Psi}{\partial x} = 0, \quad x^n \frac{\partial \varphi}{\partial x} - \Psi = 0,$$

$$\varphi(x,0) = 0; \quad \Psi(0,\tau) = A\,(t_{k+1} - \tau)/\lambda(\vartheta(0, t_{k+1} - \tau)), \qquad \Psi(1,\tau) = A\,(t_{k+1} - \tau)/\lambda(\vartheta(1, t_{k+1} - \tau)) \tag{17}$$

In conjugate problem (17), $\tau = t_{k+1} - t$ is the inverse time, and $A(t)$ is the mismatch contained in brackets in Eq. (13). The numerically differential analogues of problems (14), (2), (15) and (17) are solved by the flow run [5]. The minimization of functionals Y and Z is performed in turn until the revision of the thermal conductivity on successive iteration results in the improved result of the heat capacity determination. The heat capacity and thermal conductivity are then reconstructed simultaneously. The solution of the model problems for the determination of $C(\vartheta)$ and $\lambda(\vartheta)$ shows the good efficiency of algorithm (Figs 3 and 4).

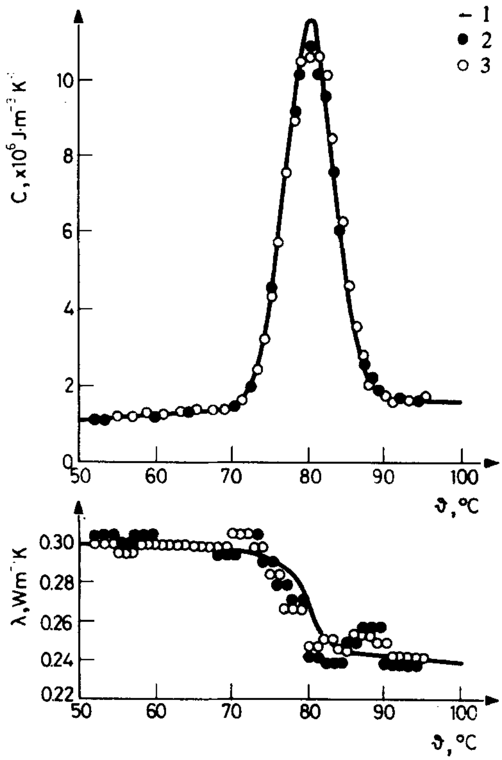

Fig. 3 Simultaneous determination of heat capacity and thermal conductivity for a plane specimen ($n = 0$): 1 – exact values, 2 – result of determination with smooth input data, 3 – solution of inverse problem with input data perturbed by first method.

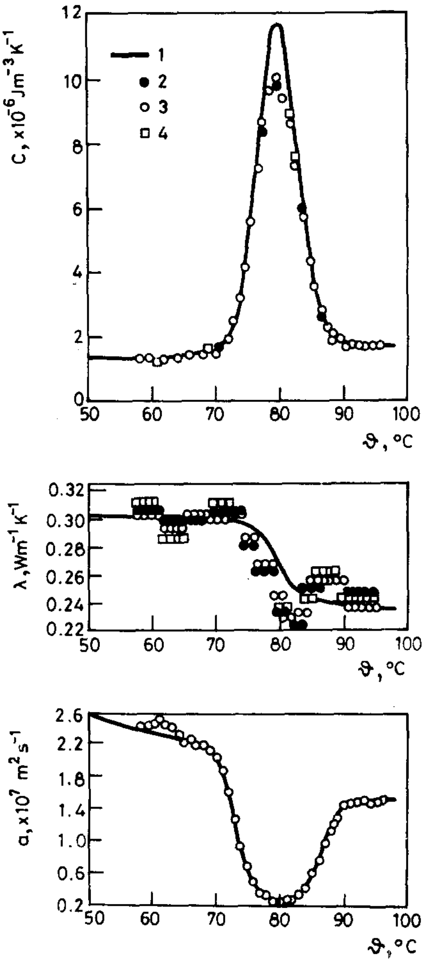

Fig. 4 Solution of inverse problem for a cylindrical specimen: 1 – exact values, 2 – with smooth data, 3 – with data perturbed by first method, 4 – with data perturbed by second method.

Since the measurements of temperature are usually carried out with an error, special numerical experiments to verify the stability of the algorithm operation have been performed. The perturbations into smooth boundary data $\vartheta_1(t)$ and $\vartheta_2(t)$ were introduced by two methods, simulating either a limitation on the sensitivity of the measuring instruments or random noise: 1) by discarding the digits to the first decimal place; 2) by adding a normally distributed random value with zero expected value. The computational experiments indicated the stability of the algorithm operation, with the error values of the input data close to the real ones (Figs 3 and 4).

Thus, the suggested algorithm can be applied for the experimental determination of the heat capacity (in the intervals of melting of the multicomponent mixtures, near the Debye temperature for crystalline materials, etc.) both for the case of a known thermal conductivity, and for the case when the thermal conductivity is unknown and should be determined simultaneously with the heat capacity.

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Zusammenfassung — Die vorgeschlagene Methode zur Bestimmung der Temperaturabhängigkeit der Wärmekapazität aus den Daten eines nichtstationären Versuchs gründet sich auf die Lösung der umgekehrten Aufgabe in einer überbestimmten Aufstellung, sie erlaubt, die Temperaturverteilung innerhalb der festen Probe in Betracht zu ziehen. Der ausgearbeitete Lösungsalgorithmus gestattet, die Wärmekapazität zu bestimmen, und zwar sowohl, wenn die Wärmeleitfähigkeit des Materials bekannt ist, als auch, wenn sie unbekannt ist und gleichzeitig mit der Wärmekapazität bestimmt werden soll. Die vorgeschlagene Methode der numerischen Lösung des Problems der inversen Koeffizienten bei der nichtlinearen Wärmeleitfähigkeit kann auch bei der Auswertung von Daten der thermischen Analyse verwendet werden.

РЕЗЮМЕ — Предложен метод численного определения температурной зависимости теплоемкости по данным нестационарного эксперимента, основанный на решении обратной задачи в переопределенной постановке и позволяющий учесть распределение температуры внутри тела. Разработанный алгоритм решения задачи позволяет определять теплоемкость как в случае известной теплопроводности материала, так и в случае, когда теплопроводность материала не известна и подлежит определению вместе с теплоемкостью. Предложенный метод численного решения коэффициентной обратной задачи нелинейной теплопроводности может быть полезен также при расшифровке данных термического анализа.