THERMOPHYSICAL PROPERTIES OF THIN METAL FILMS

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A method is proposed for determining thermophysical properties of thin metallic films, using solutions of converse thermal conductivity problems.

Various methods are known for determining thermophysical characteristics of thin films [1-3], but the most promising appear to be those based on solution of converse thermal conductivity problems [4-9]. In this technique the known boundary conditions and results of temperature measurements within the body are used to determine the unknown thermophysical quantities.

The method to be described is analogous to that of [4, 7], but differs in that the finite element method is used for solution of the direct nonlinear thermal conductivity problem. This approach is used because no problems of stability in the numerical solutions obtained develop in the case of materials with differing thermophysical characteristics.

The metal films to be studied, grown on dielectric substrates, were placed on a massive base in a vacuum cryostat [10]. The temperature coefficient of the film electrical resistance was measured first. To determine the unknown quantities shor duration (∿4 msec) rectangular pulses of dc current were passed through the specimen. Upon heating by the pulsed current the temperature regime of the deposited film can be determined by solution of the nonsteady state nonlinear thermal conductivity equation [11]:

$$C_s(T)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda_s(t)\frac{\partial T}{\partial x}\right) + Q(t),\quad \begin{matrix} 0 < x < b, \\ 0 < t < t^*. \end{matrix} \tag{1}$$

We consider heat propagation in only one direction − through the thickness of the film-substrate-base system. We assume the thermal contact between the layers ideal, i.e., we assume equality of temperatures and thermal fluxes at the layer boundaries. The following boundary conditions are specified:

$$\frac{\partial T}{\partial x}(0,\ t) = 0,\ 0 < t \leqslant t^*; \tag{2}$$

$$\lambda_{\text{base}}\frac{\partial T}{\partial x}(b,\ T) = \alpha(T - T_0),\ 0 < t \leqslant t^*. \tag{3}$$

The initial temperature of the entire system is assumed constant and equal to the temperature of the surrounding medium:

$$T(x,\ 0) = T_{\text{m}},\ 0 \leqslant x \leqslant b. \tag{4}$$

The input data for solution of the converse thermal conductivity problem are temperature measurements at one or several points, as indicated in Fig. 1:

$$T(x_i,\ t) = f_i(t),\ i = 1,\ 2,\ \ldots,\ N.$$

As a criterion for choice of the unknown characteristics we use the mean square deviation of the temperature values calculated from the mathematical model of Eqs. (1)-(4) at the points of sensor installation from the experimentally measured values:

$$J(C_s,\ \lambda_s) = \sum_{i=1}^{N}\int_0^{t^*}[T(x_i,\ t,\ C_s,\ \lambda_s) - f(x_i,\ t)]^2\,dt. \tag{5}$$

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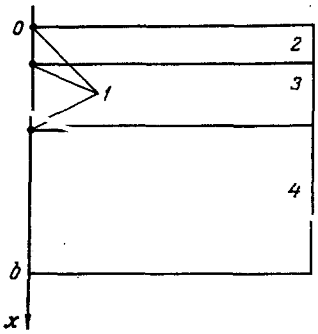

Fig. 1. Diagram of experimental method: 1) temperature sensors; 2) thin metal film; 3) dielectric substrate; 4) massive base.

Here $T(x_i, t, C_s, \lambda_s)$ are the calculated temperature values at the points x_i, i = 1, 2, 3, ..., N, obtained by solution of the initial-boundary problem, Eqs. (1)-(4): $f(x_i, t)$ are the measured temperature values of these same points, it being assumed that for the given temperature range it is known that:

$$C_{\min} \leqslant C_f \leqslant C_{\max}, \quad \lambda_{\min} \leqslant \lambda_f \leqslant \lambda_{\max}.$$

It has been established by the analysis of conditions for existence and uniqueness of the solution of the converse problem presented in [4, 9] that for unambiguous reestablishment of two thermophysical characteristics a unique solution of the converse thermal conductivity problem can be produced by temperature measurements at two separate points and specification on at least one of the boundaries of a boundary condition of the second sort. With the thermal flux density necessarily being nonzero. In our case we specify a condition of the third sort with known heat exchange coefficient and known temperature of the external medium. The unknown heat capacity and thermal conductivity coefficients of the film are approximated in the form [12]:

$$C_s(T) = \sum_{k=1}^{m} C^k \varphi_k(T), \tag{6}$$

$$\lambda_s(T) = \sum_{k=1}^{m} \lambda^k \varphi_k(T), \tag{7}$$

where C^k, λ^k are the unknown coefficients of the expansion: $\varphi_k(T)$ are first, second, and third order functions with compact carrier of the form of [12]:

$$\varphi_1 = \frac{1}{2}(1-t), \quad \varphi_2 = \frac{1}{2}(1+t), \quad \text{if} \quad m = 2,$$

$$\varphi_1 = \frac{1}{2}(1-t)\,t, \quad \varphi_2 = (1-t)(1+t), \quad \varphi_3 = \frac{1}{2}(1+t)\,t, \quad \text{if} \quad m = 3, \tag{8}$$

$$\left.\begin{aligned} \varphi_1 &= -\frac{9}{16}\left(t+\frac{1}{3}\right)\left(t-\frac{1}{3}\right)(t-1), \\ \varphi_2 &= \frac{9}{16}(t+1)\left(t+\frac{1}{3}\right)\left(t-\frac{1}{3}\right), \\ \varphi_3 &= \frac{27}{16}(t+1)\left(t-\frac{1}{3}\right)(t-1), \\ \varphi_4 &= -\frac{27}{16}(t+1)\left(t+\frac{1}{3}\right)(t-1). \end{aligned}\right\} \quad \text{if} \quad m = 4.$$

As results of processing experimental data show, the temperature dependence of thermophysical characteristics of various materials can be approximated well by polynomials of no more than third degree [7]. To find the minimum of functional (5) we use the gradient projection method [13]. Calculation of the gradient of the functional, as required by this method, is carried out by solution of the initial-boundary problem, combined with the problem of temperature increase in the film-substrate-base system. Considering the problem of Eqs. (1)-(4) as a multilayer one with number of layers greater than three, where the boundaries of layers with identical thermophysical characteristics coincide with the points of attachment of the temperature sensors, we obtain an expression for the gradient components along the unknown parameters. It is assumed that "ideal" thermal contact between layers is accomplished and contact thermal resistances are equal to zero, i.e., the conditions

$$T_i(x_{i+1},\ t) = T_{i+1}(x_{i+1},\ t),\ \frac{\partial T_i}{\partial x}(x_{i+1},\ t) = \frac{\partial T_{i+1}}{\partial x}(x_{i+1},\ t).$$

are satisifed. Following the method of [4, 7, 13] we introduce the initial-boundary problem conjugate to the problem of the change in temperature fields, of the form

$$-C_s(\psi)\frac{\partial \psi_i}{\partial t} = \lambda_s(\psi)\frac{\partial \psi_i}{\partial t},\quad \begin{matrix} 0 \leqslant x \leqslant b, \\ 0 \leqslant t \leqslant t^*, \end{matrix} \tag{9}$$

$$\psi_i(x_i,\ t^*) = 0, \tag{10}$$

$$\psi(0,\ t) = 0, \tag{11}$$

$$-\lambda_s\left[\frac{\partial \psi_{i+1}}{\partial x}(x_{i-1},\ t) - \frac{\partial \psi_i}{\partial x}(x_i,\ t)\right] = 2\left[T_{s_i}(x_i,\ t) - f_i(t)\right], \tag{12}$$

$$\psi_{i-1}(x_i,\ t) = \psi_i(x_i,\ t), \tag{13}$$

$$\lambda\frac{\partial \psi_i(b,\ t)}{\partial x} = \psi(b,\ t). \tag{14}$$

Now in a manner similar to [5, 8, 9] we obtain for the components of the gradient of functional (5):

$$\frac{\partial J}{\partial \lambda_h} = \int_0^{t^*}\left[\psi(0,\ t)\,\psi_h(T)\left.\frac{\partial T}{\partial x}\right|_{x=0} - \psi(b,\ t)\,\varphi_h(T)\left.\frac{\partial T}{\partial x}\right|_{x=l}\right]dt +$$

$$+\int_0^b\int_0^{t^*}\psi(x,\ t)\left[\frac{\partial^2 T}{\partial x^2}\varphi_h(T) + \left(\frac{\partial T}{\partial x}\right)^2\frac{\partial \varphi_h(T)}{\partial T}\right]dxdt,$$

$$\frac{\partial J}{\partial C_h} = -\int_0^b\int_0^{t^*}\psi(x,\ t)\,\varphi_h(T)\,dxdt.$$

Having obtained in explicit form the gradient of the entire functional (5), we can construct an effective algorithm for its minimization. Here we make use of the gradient projection method of [13]. In the given case this reduces to construction of a minimizing sequence of the form:

$$Z_{k+1}\begin{cases} P_k, & Z_{\min} \leqslant P_k \leqslant Z_{\max}, \\ Z_{\min}, & P_k < Z_{\min}, \\ Z_{\max}, & P_k > Z_{\max}, \end{cases} \tag{15}$$

where

$$P_k = \lambda_k - \beta_k J'_\lambda \quad \text{or} \quad P_k = C_k - \beta_k J'_c. \tag{16}$$

The descent parameter β is chosen by using the one-dimensional optimization method. Consequently, the algorithm constructed for finding the functions λ(T) and C(T) consists of the following. A number of equidistant nodes m are specified for interpolation of the unknown functions by polynomials of the form of Eq. (8) over the interval $[T_{min}, T_{max}]$, which is determined beforehand. Then initial values are chosen for the unknown coefficients $\{\lambda_s, C_s\}$ just as in the case of massive bodies, and the problem of Eqs. (1)-(4) is solved numerically. From the temperature field T(x, t) found in this manner and appearing in the boundary conditions, for the conjugate problem of Eqs. (15), (16) we find the minimum of functional (5) in the given direction by the golden section method. The values obtained for $\{\lambda_s, C_s\}$ are used as an initial approximation for the following iteration. The process is terminated when:

$$\sum_{i=1}^{m} \int_0^{t^*} [T_{s_i}(x_i, t) - f_i(t)^2]\, dt \simeq \delta^2,$$

where $\delta^2 = \sum_{i=1}^{n} \int_0^{t^*} \sigma_i dt$ is an estimate of the generalized uncertainty of the initial data, σ_i is the mean square deviation of the input data at the points $x = x_i$ at time t.

The algorithm described above was realized in the form of a Fortran program for an ES computer. In solving the nonlinear thermal conductivity problem the Krank–Nicholson–Galerkin method [14] and the finite element method with second order approximation were used. Use of the semidiscrete approximations:

$$T_n(x, t) = \sum_{i=1}^{N} Q^i(\tau)\varphi_i(x)$$

transforms the solution of the initial-boundary problem, Eqs. (1)-(7), to a solution of the Cauchy problem for a system of nonlinear differential equations of the form:

$$(C(T_n)\dot{T}_n, \psi_i) + a(T_n, T_n, \psi_i) - \alpha T_n \psi_i = (W, \psi_i) + \alpha T_c \psi_i, \quad (17)$$

$$(T_n, \psi_i)_{\tau=0} = (T_0, \psi_i), \; i = 1, 2, 3, \ldots, N. \quad (18)$$

Here the notation $[\dot{T}_n = \partial T_n/\partial t$ has been introduced and it is considered that $\partial T_n/\partial T \in L_2[0, t^*]$, $(\cdot, \cdot)$ – the scalar product in $L_2(0, b)$:

$$(u \cdot v) = \int_0^b u \cdot v dx, \; a(T_n, T_n, \psi_i) = -\int_0^b \lambda(T_n) \frac{\partial T_n}{\partial x} \frac{\partial T_n}{\partial x} dx.$$

Now, writing Eqs. (17) and (18) in matrix form, we obtain:

$$M(Q)\dot{Q}(t) + G(Q)Q(t) = F(t), \quad (19)$$

$$Q(0) = r. \quad (20)$$

Let $t_m = M\Delta t$, $\Delta t = t^*/M$, where M is an integer and $F_m = F(\tau_m)$; $Q(t) = \sum_{i=1}^{2} q_i \chi_i(t)$, were $X_i(t)$ are linear base functions. Then the Cauchy problem for the system of nonlinear differential equations (19)-(20) reduces to solution of the system

$$M(q_{m+\frac{1}{2}}) \frac{q_{m+1} - q_m}{\Delta t} + G(q_{m+\frac{1}{2}}) = F_{m+\frac{1}{2}}. \quad (21)$$

Here $q_{m+\frac{1}{2}} = \theta q_{m+1} + (1-\theta) q_m$, where $0 \le \theta \le 1$, while $F_{m+\frac{1}{2}} = \theta F_m + (1-\theta) F_m$.

To find the vector q_m we must solve the system of nonlinear algebraic equations, Eq. (21), for each step in time. To avoid iteration procedures of the Newton–Kantorovich method type, we use a predictor-corrector algorithm. In each time step we must then solve two systems of nonlinear algebraic equations:

$$M(q_m) \frac{\beta_{m+1} - q_m}{\Delta\tau} + G(q_m) q_m = F_{m+\frac{1}{2}}(q_m),$$

$$M\left(\frac{\beta_{m+1} + q_m}{2}\right) \frac{q_{m+1} - q_m}{\Delta\tau} + G\left(\frac{\beta_{m+1} - q_m}{2}\right) q_m = F_{m+\frac{1}{2}}\left(\frac{\beta_{m+1} + q_m}{2}\right).$$

A similar method is used for solution of the conjugate problem in Eqs. (9)-(14). Thus a quite general algorithm has been proposed for determining thermophysical characteristics of materials – heat capacity and thermal conductivity. The case in which one of the characteristics is known decreases the minimum number of sensors for temperature measurement, while the algorithm remains unchanged. To check the software developed a test problem of reconstructing the thermal conductivity coefficient of a thin film was considered. On the whole the mathematical testing performed showed the effectiveness of the approach described for determining thermophysical characteristics of thin films.

NOTATION

T(x, t), temperature at point x; t, times; $C_S(T)$, $\lambda_S(T)$, heat capacity and thermal conductivity coefficients; α, heat exchange coefficient; T_0, temperature of external medium; Q(t), specific power of heat sources.

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DETERMINATION OF THERMAL CONTACT RESISTANCES USING THE SPECTRAL FUNCTIONS OF BOUNDARY EFFECTS

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A method is proposed for determining thermal contact resistances by solving the inverse heat-conduction problem.

The growing requirements for the design of economical heat machines cannot be satisfied without knowledge of the heat processes occurring in them. The study of heat-exchange processes involves a full-scale thermophysical experiment which provides information about the temperature field from a limited set of observation points, located inside the machine; this information is then used to solve the inverse heat-conduction (IHC) problem in order to find the boundary effects, which are necessary for determining the thermally stressed state of the parts and units of heat machines.

It is of particular interest to determine boundary conditions of the fourth kind, i.e., the thermal contact resistances (TCR's) between the surfaces of the parts in contact, with the aid of the solution of the IHC problem from the results of a thermophysical experiment.

The dynamics of the thermal process for a composite body is described by the heat equation

$$\frac{\partial}{\partial x}\left[\lambda(x,\ y,\ T)\frac{\partial T}{\partial x}\right]+\frac{\partial}{\partial y}\left[\lambda(x,\ y,\ T)\frac{\partial T}{\partial y}\right]=c_V(x,\ y,\ T)\frac{\partial T}{\partial t}. \tag{1}$$

Besides Eq. (1), the mathematical model (of the phenomenon under consideration) determining the thermal state of the object also contains the initial edge conditions

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