# PLANNING A PHYSICAL EXPERIMENT ON DETERMINATION OF THE PARAMETERS OF A MATERIAL BY USING MATHEMATICAL METHODS

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A method is developed for solving an inverse problem on the determination of thermomechanical parameters of a material that undergoes phase transformations in the process of hardening. The dependence of the error of determination of parameters on the error admissible in direct measurements of physical fields is established.

1. The use of mathematical simulation of the processes of structurization in metals and alloys during thermal treatment as an instrument of optimization of the complex of controlling paramters is finding ever-increasing use. An application of an ideal mathematical model is related to completeness of information on physical properties of the material. However, the possibilities of an experimental determination of thermophysical and mechanical properties available are limited as present, especially because structure in steels in thermal processing forms under stresses that considerably affect the distribution of structural components and, consequently, the ultimate properties of the material. Therefore, solving inverse problems, such as interpreting the data of a physical experiment [1-3], is an effective technique for obtaining information on thermophysical and mechanical parameters. Since problems of this class are "incorrect" problems, regularizing algorithms are used for their solution [4].

Since any physical experiment is related to measurement errors, the estimate of the influence of these errors on the quality of the solutions obtained and also on the accuracy of determination of one or another parameter seems to be very important. The determination of this kind of estimate and, correspondingly, the solution of the problem on planning an experiment on measurement of physical fields as input data of the inverse problem under consideration constitute the purpose of the present work.

2. The model of thermal treatment that we accepted is related to inductive heating of steel cylindrical samples for hardening [5]. Thermomechanical effects are considered on the basis of the theory of plastic flow [6], where the corresponding solution includes both thermal and structural components of the stress tensor. The latter is significant since the model contains both the estimates of the inverse effect of stresses on structural transformations and the effect of structure on the thermal field T.

Therefore, the physical process is described by an initial-value boundary-value problem for a self-adjoint evolving system of partial differential equations that includes a nonlinear equation of heat conduction with conditions of convective heat exchange and radiation on the boundary of a cylinder with the Maxwell equations in a quasistationary approximation (in the stage of inductive heating) and nonlinear equations for calculating the field of stresses and deformations.

The effect of stresses on a thermal field in the process of hardening is considered with the help of the following expression for the speed of the latent heat liberation for a phase transformation:

$$\dot{Q} = \sum_i q_i \dot{\xi}_i,$$

where i is the corresponding phase transition number, $q_i$ is the latent heat of transition, and $\xi_i$ is the partial volume of the i-th phase.

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Accordingly, the system is closed by integral representations for the volumetric parts of different crystal phases that are formed in the process of rapid cooling. In the given work, the process of the complete decomposition of austenite $\xi_3$ into perlite $\xi_1$ and martensite $\xi_2$ is considered:

$$\xi_1 = \left\{1 - \exp\left[-\varkappa \int_{t_0}^{t} \left(\frac{T-720}{195}\right)^2 \left(\frac{T-380}{145}\right)^2 \exp(p\bar{\sigma})(t-\tau)^3 d\tau\right]\right\},$$

$$\xi_2 = (1-\xi_1)\{1 - \exp[\Phi(300-T) + A\bar{\sigma} + B\sigma_i]\},$$

$$\xi_3 = 1 - \xi_1 - \xi_2.$$

In this case, $\xi_1$ is calculated only in the temperature range 380°C ≤ T ≤ 720°C; for T > 720°C, we have $\xi_1 = 0$, and the formation of the perlite structure is terminated for T < 380°C. The situation is similar for $\xi_2$ in the temperature range 100°C ≤ T ≤ 300°C. In these equations $\varkappa$, p, $\Phi$, A, and B are constants determined by the steel grade; $\bar{\sigma}$ are the average stresses, $\bar{\sigma} = 1/3$ tr $\sigma_{ij}$; $\sigma_i$ are the stress intensities; T is the temperature field; and $t_0$ is the initial moment of hardening.

These equations reflect the Jones–Mell hypothesis [7, 8] with the adjustment on nonisothermality of the process of decomposition of austenite and with account of the effect of stresses on decomposition under certain simplifying assumptions.

The described system of equations, solvable by an iterational difference method similar to [5, 9] serves as a basis for the program-sensor of three physical fields: a temperature field, a stress and deformation field, and a distribution field for the structural components. These fields, therefore, are algorithmically defined on a spatial–temporal mesh for any set of physical parameters of the material and process.

Let us refer to the description of these parameters.

3. When cooling is rapid, we can neglect the dependence of the thermophysical parameters on temperature [5]. On the other hand, there is evidence that in the framework of a model exhibiting mutual interaction of physical fields, it is necessary to distinguish between the phenomenological characteristics of crystalline phases [8]. In connection with this, we are interested in the following parameters: the heat conduction of each phase $\lambda_i(T)$, the volumetric expansion coefficient $\alpha_i(T)$, and the parameter p responsible for the formation of the perlite structure from the inner stresses in the sample.

We note that since the microstructure of the material is not ordered, parameters of the mixture that enter into equations of heat conduction and thermoelastoplasticity at each moment t and at each point of the sample r are described by the equations

$$\lambda(r, t) = \sum_i \xi_i(r, t)\lambda_i(T), \quad \alpha(r, t) = \sum_i \xi_i(r, t)\alpha_i(T)$$

(the representations $\xi_i$ are given above). In our mathematical model $\lambda_1$, $\lambda_2$, $\alpha_1$, and $\alpha_2$ do not depend on temperature: $\lambda_3(T)$ and $\alpha_3(T)$ are linear functions of temperature, the values of which at one of the points (for example, for T = 850°C) are known from the reference literature [10], so that these functions are defined uniquely by the values (for example, for T = 20°C) of $\lambda_3$ and $\alpha_3$.

Therefore, the desired vector is the vector $\mathbf{p} = \{\lambda_1, \lambda_2, \lambda_3, \alpha_1, \alpha_2, \alpha_3\}$, the values of which we choose from the compact set defined by the information on maximal and minimal values of the parameters for the given steel grade [8, 11]: $\tilde{\lambda} \le \lambda_i \le \tilde{\tilde{\lambda}}$, $\tilde{\alpha} \le \alpha_i \le \tilde{\tilde{\alpha}}$, $\tilde{p} \le p \le \tilde{\tilde{p}}$ $(i = \overline{1, 3})$. Below, we denote the indicated set as $\Omega_p$.

4. By means of a physical experiment related to the specific technology of cooling of a sample on the given spatial–temporal mesh, the fields $T_e(r_i, t_j)$ can be obtained in the course of the process, and the values of $\sigma_{\theta\theta}{}^e(r_i, t_j)$, $\xi_1{}^e(r_i, t_j)$ at the moment of its completion $\hat{t}$. They can serve as indirect information for determining p so that the deviation of the "calculated" field from the experimental field is a minimum.

Since p is selected from the compactum $\Omega_p$, such a problem corresponds to the concept of quasisolution [4], where the closure measure for the observed and calculated values is

determined in a certain compact space. However, since the sensitivity of the deviations of different fields to different parameters is different, it is convenient to elaborate on the problem formulation and at the same time to define an effective algorithm for solving the problem.

We introduce the functionals

$$\Phi_1[\mathrm{p}] = \int_0^R \int_{t_0}^{\hat{t}} \gamma_1 [T(r, \tau, \mathrm{p}) - T_e(r, \tau)]^2 \, d\tau dr;$$

$$\Phi_2[\mathrm{p}] = \int_0^R [\gamma_2 |\sigma_{\theta\theta}(r, \hat{t}, \mathrm{p}) - \sigma^e_{\theta\theta}(r, \hat{t})|^{\frac{1}{2}} + \gamma_3 |\xi_1(r, \hat{t}, \mathrm{p}) - \xi^e_1(r, \hat{t})|] \, dr,$$

where $\gamma_1$, $\gamma_2$, and $\gamma_3$ are weighted factors introduced taking account of the difference in the dimensionality of functionals ($\gamma_i = 1/|\Phi_i|$, $i = \overline{1, 3}$); R is the sample radius.

As a minimizing algorithm, an iterative method of quickest descent has been chosen on different groups of parameters for different functionals. It consists of two stages. At the first stage the set is constructed on which the functional $\Phi = \Phi_1 + \Phi_2$ has a unique minimum, coinciding with the global minimum. In order to do this, a certain sequence of values is specified: $\{p_k\} \subset [\tilde{p}, \tilde{\tilde{p}}]$. For each of these $p_k$ for the given initial value of $q^{(0)} = \{\lambda_1^{(0)}, \lambda_2^{(0)}, \lambda_3^{(0)}, \alpha_1^{(0)}, \alpha_2^{(0)}, \alpha_3^{(0)}\}$, an iteration process is realized, which is completed when the following conditions hold:

$$|\lambda_i^{(s)} - \lambda_i^{(s-1)}| < 10^{-3} |\lambda_i^{(s-1)}|, \; |\alpha_i^{(s)} - \alpha_i^{(s-1)}| < 10^{-3} |\alpha_i^{(s-1)}|;$$

we denote the result of this process by $q_k$.

Each step of this process includes two variational procedures: from the given $\alpha^{(s-1)} = \{\alpha_1^{(s-1)}, \alpha_2^{(s-1)}, \alpha_3^{(s-1)}\}$ by minimization of $\Phi_1$ with respect to $\lambda$, we obtain $\lambda^{(s)} = \{\lambda_1^{(s)}, \lambda_2^{(s)}, \lambda_2^{(s)}\}$; with respect to $\lambda(s)$ by minimization of $\Phi_2$ we obtain $\alpha^{(s)}$.

As a result of the interation process, a set of minimal values of $\{\Phi^{(k)}\}$ is obtained, from which we select

$$\hat{\Phi} = \min_k \Phi^{(k)}$$

and the corresponding

$$\mathrm{p}_{k_0} = \{q_{k_0}, p_{k_0}\}.$$

As the desired set, which contains the global minimum point, the segment $[p_{k-1}, p_{k+1}]$, which replaces the given set $[\tilde{p}, \tilde{\tilde{p}}]$, is taken. The determined value of $p_{k_0}$ is assumed to be an initial approximation for the algorithm of the next stage.

At the second stage, the purpose of which is solving the following problem of quasiminimization for the given "allowances" $\delta_1$ and $\delta_2$:

$$\Phi_1[\mathrm{p}] \leqslant \delta_1, \quad \Phi_2[\mathrm{p}] \leqslant \delta_2,$$

in the neighborhood of the global minimum, the following iteration process is realized. From $\lambda^{(j-1)} = \{\lambda_1^{(j-1)}, \lambda_2^{(j-1)}, \lambda_3^{(j-1)}\}$ by minimization of $\Phi_2$ with respect to $\{\alpha_1, \alpha_2, \alpha_3, \mathrm{p}\}$ the quantity $r^{(j)} = \{\alpha_1^{(j)}, \alpha_2^{(j)}, \alpha_3^{(j)}, \mathrm{p}^{(j)}\}$, is determined; from the $r^{(j)}$ determined by minimization of $\Phi_1$ with respect to the set $\{\lambda_1, \lambda_2, \lambda_3\} - \lambda^{(j)}$. The process is completed under the same condition as above.

For the case when the condition of quasiminimization does not hold, the process is repeated, however, on a smaller mesh with respect to p. The results, given below, prove that such an algorithm is effective.

5. We direct our attention to the results of a numerical experiment.

Initially, as "experimental" data, the physical fields $\{T, \sigma_{\theta\theta}, \xi_1\}$ were considered, calculated in advance from the given $p_0$ with computer accuracy. From these fields the value of p was reconstructed with accuracy up to 0.1%, which demonstrates clearly the efficiency of the selected algorithm.

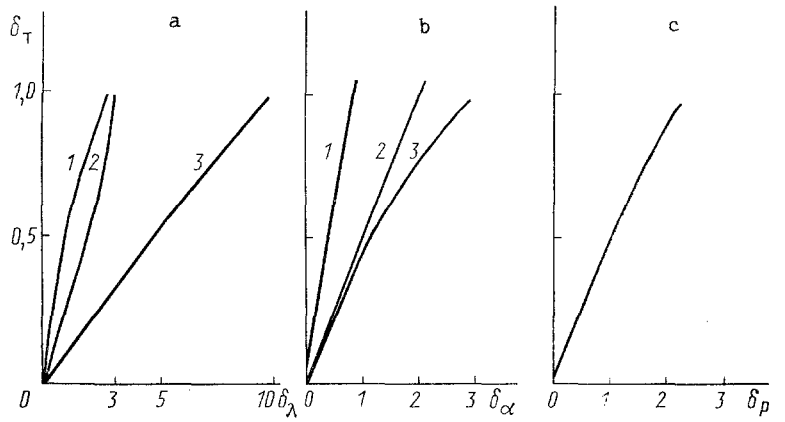


Fig. 1. Dependence of the relative error in determination of the temperature $\delta_T$ on the relative error of parameters $\lambda$ (a), $\alpha$ (b), p (c) for $\delta_\xi = 0\%$, $\delta_\sigma = 0\%$: 1) perlite; 2) martensite; 3) austenite. $\delta_T$, $\delta_\lambda$, $\delta_p$, %.

Next, we were interested in the dependence of an error of the results obtained on the error of measurement of physical fields. Since the inverse problem is incorrect, the a priori estimates of this error are impossible, and, therefore, the a posteriori estimates, obtained on the basis of a special mathematical experiment [1, 4], serve as their alternative. For this purpose we use perturbated simulating fields, where the relative error at the level $\delta$ (%) is simulated by the following equations:

$$T_e = T(1 \pm 10^{-2}\delta_T), \quad \sigma^e_{\theta\theta} = \sigma_{\theta\theta}(1 \pm 10^{-2}\delta_\sigma), \quad \xi^e_1 = \xi_1(1 \pm 10^{-2}\delta_\xi).$$

Then from the fields perturbated in this way, we reconstructed the parameter p (preserving stability due to the correctness of our problem formulation), and its value was compared to the initial one. The deviation of p from the initial $p_0$ is estimated from the relative deviation of each vector component

$$\delta_{p_i}(\%) = \frac{|p_i - p_{0i}|}{|p_{0i}|} 100\%$$

and serves as a measure of the error of the result.

The data obtained can serve as an important factor for planning experimental measurements. Hence it follows that:

1. The most substantial effect on the determination of parameters of heat conduction $\lambda_i$ is produced by the error in the measurement of the thermal field. The surpassing of the relative error in the determination of this field by more than 1% results in a more than 10% error in the determination of $\lambda_i$ (Fig. 1a), while an error in the determination of the structural field of up to 10% and an error in the stress field of up to 20% (Figs. 2a and 3a) produce a weak effect on the relative error in the determination of $\lambda_i$, less than 1%.

2. The use of the information on distribution of the structural field in the determination of parameters $\{\lambda_i, \alpha_i, p\}$ leads to the result that the measurement of the stress field with a relative error up to 20% allows us to determine parameters with relative error up to 3% (Fig. 2). This is an interesting result since an experimental determination of stresses with relative error lower than 10-15% requires local destructive methods and bulky statistical processing of experimental data.

3. The error in the measurement of the structural field influences noticeably an error in the determination of the parameters (Fig. 3). Since the experimental determination of the structural component with the relative error below 5% requires considerable time expenses and the use of expensive equipment, in practice, the main goal should be determined and the labor involved in the experiment to achieve this goal should be minimized, or a compromise should be sought between the computational and experimental work. In Fig. 3, the results are represented closest to the possibilities of the contemporary experimental base $\{\delta_T = 0.5\%, \delta_\sigma = 10\%\}$ that allow us to judge on the influence of $\delta_\xi$ on the accuracy of the determination of parameters.

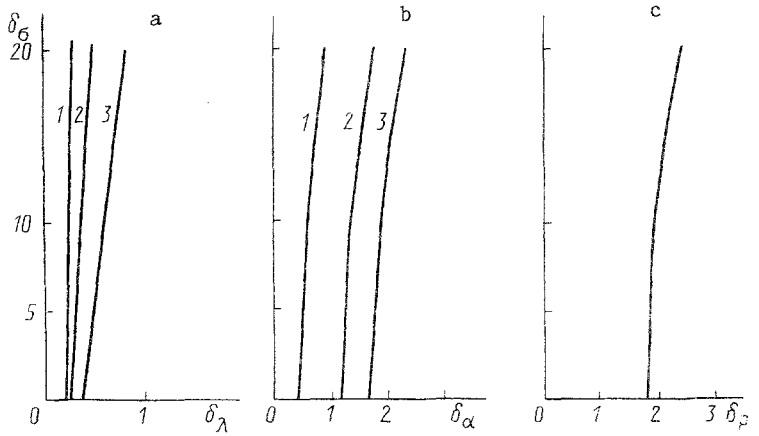


Fig. 2. Dependence of the relative error in determination of stresses $\delta_\sigma$ on the relative error of the parameters $\lambda$ (a), $\alpha$ (b), p (c) for $\delta_T$ = 0%, $\delta_\xi$ = 3%: 1) perlite; 2) martensite; 3) austenite. $\delta_\sigma$, %.

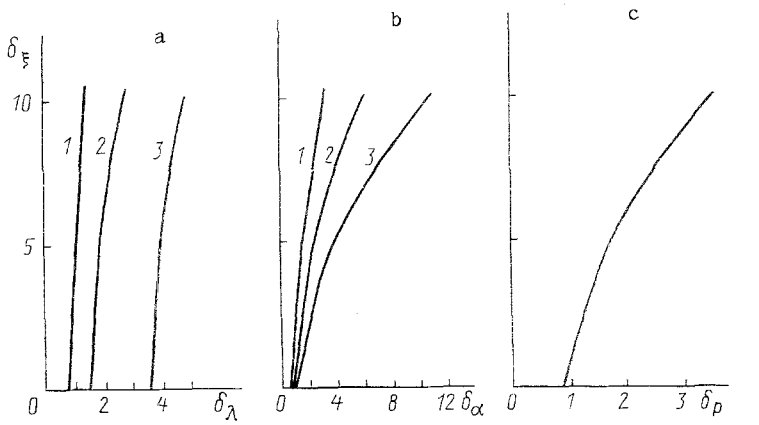


Fig. 3. Dependence of the relative error in the determination of the structural component $\delta_\xi$ on the relative error of the parameters $\lambda$ (a), $\alpha$ (b), p (c) for $\delta_T$ = 0.5%, $\delta_\sigma$ = 10%: 1) perlite; 2) martensite; 3) austenite.

Therefore, these investigations work out the strategy of conducting a physical experiment on the measurement of the group of values: T, $\sigma_{\theta\theta}$, $\xi_1$ and can serve as a basis for the automated system of determination of physical parameters of structural components for the given grades of steel with the influence of the stress field and structural transformations clearly defined.

In the framework of the described methodology one can use an even more complete model of structural transformations. Also other (including functional) parameters of the material or process can be the goal of the search.

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# CONTROLLED RATIONAL HEATING OF OBJECTS FOR HEAT TREATMENT

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The article presents a method of solving the problem of controlled heating involving the reproduction of some regularity of heating the surface of an object. As an example the article presents the solution of the problem of controlled radiative heating of a steel cylinder, and the obtained calculation is compared with experimental data.

The heating of steel is a widely used operation in processes of heat treatment such as annealing, tempering, normalization, and hardening. The quality and conditions of heating largely determine the subsequent properties of parts subjected to heat treatment. The heating temperature of different marques of steel lies in a wide range from 20 to 1300°C, and heating itself is carried out at different rates. Different heat sources are therefore used: electrical, radiative, plasma, lasers, electron beams. As a rule, a certain power is established which is used during the entire heating process. The heating rate is not varied in different temperature ranges, and power expenditure on heating is not being optimized. Yet in some cases it is necessary to ensure a variable heating rate at different stages of heating. This can be done by controlling the intensity of the supplied power ensuring the required temperature regime.

In the general case the problem of external heating can be formulated in the following way: we have to heat some object in such a way that its surface is heated according to the previously specified regularity $T_s = f(\tau)$. For that we have to find such a dependence $T_{so} = T_{so}(\tau)$, that the regularity $T_s = f(\tau)$ is fulfilled.

In this case the equation of heat conduction has the form [1]

$$c_p(T)\,\rho(T)\frac{\partial T}{\partial \tau} = \operatorname{div}(\lambda(T)\operatorname{grad} T) \tag{1}$$

with the boundary condition on the surface

$$\lambda(T)\frac{\partial T}{\partial \bar{n}} = \varphi(T_{so}), \tag{2}$$

where $\bar{n}$ is the outer normal to the surface of the object; $\varphi$ is some function whose form depends on the method of heating. It can be seen from the boundary condition (2) that if the function $\varphi(T_{so})$ has an inverse, and we know the dependence of $\partial T/\partial n$ on time, we can find the temperature of the source

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