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A method for calculating the temperature fields of the elements of the quantron and the structure and characteristics of the complex of programs for automated design of solid-state lasers are described.

Automation of the design of solid-state lasers is an effective way to reduce the development time of these devices. Because the thermal conditions in quantrons significantly affect the characteristics of laser radiation [1-4] special attention must be devoted to the physical and mathematical modeling of heat-transfer processes in quantrons, to the methods of their numerical realization and corresponding program complexes. These questions are examined in this paper.

There are many works devoted to the calculation of the thermal conditions in quantrons and their separate elements [2, 5-8]. However, the need for improving laser technology makes it necessary to develop the research further. Pumping systems with natural and combined cooling, operating in diverse temporal regimes at high temperatures, to obtain which a number of new solutions to structural design problems are employed [9, 10], are now widely used. This makes it necessary to carry out calculations using several numerical schemes. In addition, experience in carrying out engineering calculations shows that further simplifications must be made in the procedure of transferring from the parameters of the real structure to the starting data for the simulation programs.

Thermal and Mathematical Models. The most widely used designs of quantrons are described in [4, 7, 9, 10]. Figure 1 shows two typical designs with single-block and field reflectors. In [7] the thermal regime of a quantron is studied taking into account the thermal interaction of different elements, and the corresponding thermal and mathematical models as well as the procedure for performing the numerical calculation based on an explicit scheme are proposed. In this paper we examine a more complicated model, which gives a better approximation to the real heat-transfer process. We shall discuss its characteristic features.

The thermal model of the quantron consists of a system of thermally intercoupled bodies, in which heat propagation occurs by conduction. For some bodies, for example, the active element, the single-block or hollow reflector, three-dimensional temperature fields are studied, while for others, for example, flashlamps, the housing of the quantron, in a number of other cases fields with lower dimensionality, down to uniform fields, can be studied.

The generatrices of all cylindrical surfaces of the elements of the quantron are parallel to the same straight line — the axis of the quantron. They can be divided into two groups, depending on the geometric shape of the section of the cylindrical surfaces of the elements by a plane perpendicular to the axis of the quantron. The first group consists of elements whose section is circular or annular. This group includes active elements, some types of tubes enclosing the active element, and hollow reflectors and envelopes of flashlamps. The second group consists of elements whose section has a noncanonical shape, for example, single-block reflectors.

The thermal conductivity and specific heat capacity of materials can vary substantially as a function of the temperature of the elements of the quantron. For example, the thermal conductivity of leucosapphire, from which the single-block reflectors are fabricated, varies from 40 W/(m·K) at 20°C to 20 W/(m·K) at 200°C. For this reason in the thermal model the temperature dependences of the thermal conductivity and specific heat capacity are taken into account.

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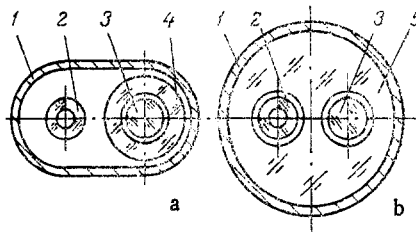


Fig. 1. Examples of the constructions of quantrons with hollow (a) and single-block (b) reflectors: 1) housing; 2) flashlamp; 3) active element; 4) leucosapphire tube; 5) single block.

During the operation of a laser, volume and surface absorption of radiation from the flashlamp, described by the multidimensional distributions of the volume and surface heat-flux density, occurs in the elements of the quantron. The temperature in the quantron in most cases is substantially nonstationary. This is determined by the operating mode of the laser in series of pulses, in which the time intervals in the presence of lasing pulses alternate with the time intervals without lasing. In the thermal model the multidimensional spatial and corresponding time-dependent distributions of the volume and surface heat sources are taken into account.

Heat exchange between the quantron and the surrounding medium and neighboring bodies is realized from the exterior side of the housing and the surfaces of other elements protruding from the housing. The conditions under which such heat exchange occurs are determined by the characteristics of the construction and operation of the optoelectronic system in which the quantron is employed. External heat exchange of the quantron is analyzed based on the corresponding thermal and mathematical models with the help of the method of stage-wise modeling [11, 12]. This approach permits taking into account in the analysis of the internal heat transfer in the quantron the external thermal effects fixed through the corresponding spatial-temporal distributions of the heat fluxes, heat transfer coefficients, and temperatures of the surrounding medium and bodies. In this work we analyze only the internal heat transfer in the quantron.

Heat is transferred between the elements of the quantron by heat conduction, radiation, and convection. The contribution of each mechanism to the total heat transfer depends strongly on the construction and the method employed for cooling the quantron.

Heat transfer by means of conduction makes an important contribution to heat transfer between elements in quantrons without forced cooling with hollow or single-block reflectors, when there is no convection in the space between elements. This condition holds for air gaps with a thickness of the order of 1-2 mm and smaller, which occurs in most cases. In describing this heat transfer in narrow annular channels the heat flux density vector is assumed to be perpendicular to the surfaces of the elements, while heat transfer along the channel is not taken into account. When taking into account the heat transfer by means of conduction in channels with a complex shape, characteristic for hollow reflectors, the corresponding multidimensional heat-conduction equation for a stationary gaseous-medium is employed.

When taking into account heat transfer by radiation the surfaces of the elements are assumed to be grey, diffusely reflecting, and emitting. In cavities with complex shapes, characteristic for hollow reflectors, it is described in the three-dimensional approximation [13].

The form of the model of convective heat transfer depends on the method employed for cooling the quantron. In systems with forced cooling the coolant usually flows in annular channels, arranged around the heating elements, in the direction of the axis of the quantron. In this case the time-dependence of the temperature of the coolant at the inlet to the channel is assumed to be fixed. It is determined from a calculation of the entire cooling loop of the quantron. Heat exchange between the coolant and the surface of the element is described on the basis of the approximation of the combined problem [20] under the condition that the coefficient of heat transfer and the temperature of the coolant change only along the length of the channel. In many cases it may be assumed that the change in the coolant temperature is linear in the direction of motion of the coolant. In describing free-convection heat transfer in the cavity of the reflector multidimensional distributions of the heat-transfer coefficients are employed. Calculations show that in this case the relations for heat trans-

fer in an unbounded space can be employed to determine the heat-transfer coefficients. At the same time the temperature of the gaseous medium, which appears in these relations, is determined from the condition of heat balance, written down for all sections into which the surfaces of the elements are divided.

Thus the mathematical model consists of a system of nonlinear multidimensional nonstationary heat-conduction equations for the elements of the quantron:

$$\rho_i c_i(T_i) \frac{\partial T_i}{\partial \tau} = \text{div}(\lambda_i(T_i) \text{grad} T_i) + q_{vi}(\bar{x}, \tau), \quad (1)$$

$$T_i|_{\tau=0} = T_{0i}(\bar{x}), \quad i = 1, 2, \dots, m, \quad (2)$$

and the energy equations for the coolants moving in the channels:

$$\rho_j c_j(T_j) \left( \frac{\partial T_j}{\partial \tau} + v_z \frac{\partial T_j}{\partial z} \right) = \sum_i \alpha_i(z, T_j, T_i) (T_j - T_i) L_i, \quad (3)$$

$$T_j|_{\tau=0} = T_{0j}(z), \quad T_j = T_{j,\text{in}}(\tau), \quad j = m+1, m+2, \dots, l, \quad (4)$$

where the  $z$  axis coincides with the axis of the quantron.

The boundary conditions for (1) have the form

$$\begin{aligned} -\lambda_i(T_i) \frac{\partial T_i}{\partial n} \Big|_{\Gamma_i} &= \sum_{\substack{v=1 \\ v \neq i}}^m \alpha_{kv}(\bar{x}_i, T_1, T_2, \dots, T_m) (T_i - T_v) + \\ &+ \sum_{\substack{v=1 \\ v \neq i}}^m \int_{S_v} \beta_{qv}(\bar{x}_i, \bar{x}_v) (T_i^4 - T_v^4) dS_v + \sum_{v=m+1}^l \alpha_v(z, T_i, T_v) (T_i - T_v) + \sum_{v=l+1}^M \alpha_v(\bar{x}_i, T_i, T_v) (T_i - T_v) + q_{Si}(\bar{x}_i, \tau), \end{aligned} \quad (5)$$

where the first and second sums on the right side describe, respectively, the convective-conductive and radiant heat transfer between the elements of the quantron; the third sum describes convective heat transfer between the surfaces of the elements and the coolants; and, the fourth sum describes the external heating effects on the elements of the quantron, determined at preceding stages of the analysis of the thermal state of the optoelectronic system. In many cases the surfaces of some elements of the quantron are coated with film heaters, with whose help the temperature of these elements can be controlled. The last term on the right side of Eq. (5) takes these heaters into account.

Numerical Computational Procedure and the Structure of the Program Complex. Inadequate attention is devoted in the literature [14, 15] to the methods employed for constructing the difference equations for systems of the type (1)-(5), their analysis, and methods of solution. Therefore, the procedure for determining the type of difference scheme is based largely on computer experiments. As a result of such studies explicit and mixed schemes were selected and implemented [16, 17]. In the mixed scheme the temperature field of each element and coolant is found using the implicit scheme, while information about the thermal effect of the bodies is taken from the preceding time layer. The desirability of employing explicit and mixed schemes is also confirmed by calculations performed in [16, 17]. With the help of such calculations it is possible to select an explicit or mixed scheme for a given specific case, taking into account the construction of the quantron and the thermophysical properties and geometric dimensions of the elements and the values of the heat-transfer coefficients.

The use of such schemes made it possible to employ the modular principle for the construction of the computing programs for specific constructions of quantrons [18], for which these programs are assembled from prepared modules of three types.

Modules of the first type implement the explicit and implicit schemes for solving heat-conduction equations, corresponding to separate elements of the quantron using different spatial grids, and an implicit scheme for solving the energy equation. The quantron is divided along the entire axis by planes perpendicular to it. For elements whose sections by a plane perpendicular to the axis of the quantron have a canonical shape, in this section the corresponding regular grid in rectangular or cylindrical coordinate system or an irregular tri-

angular grid is employed. If the shape of the cross section of the element is not canonical. An irregular triangular grid is employed and the spatial operators are approximated based on the method of finite elements [19]. In the calculation based on the implicit scheme for bodies with a canonical shape a locally one-dimensional scheme was employed [15], while in the case of an irregular grid the separation was made only along the coordinate varying along the axis of the quantron.

Modules of the second type implement algorithms for taking into account the thermal interaction of the elements of the quantron by means of radiation and convection. For example, for radiative heat exchange in cavities with complex shapes the resulting radiant heat flux  $q_{kl}^{ij}$  between the  $l$ -th and  $k$ -th sections of the surfaces of the  $i$ -th and  $j$ -th elements  $\Delta S_k^{(i)}$  and  $\Delta S_l^{(j)}$  is calculated according to the formula [20]:

$$q_{kl}^{ij} = \sigma \epsilon_{re kl}^{ij} \varphi_{kl} ((T_k^i)^4 - (T_l^j)^4) \Delta S_k^{(i)}, \quad (6)$$

where the reduced emissivities  $\epsilon_{re kl}^{ij}$  are found by solving the corresponding system of algebraic equations. In the corresponding program module the irradiance coefficients, the reduced emissivities, and the resulting heat fluxes are calculated for fixed spatial separation and configuration of the cavity. For heat transfer by convection in cavities with a complex shape the resulting convective heat flux  $q_k^{(i)}$  to the  $k$ -th element of the surface of the  $i$ -th element of the quantron  $\Delta S_k^{(i)}$  is calculated using the formula

$$q_k^{(i)} = \alpha_{ih} (T_h^{(i)} - T_c) \Delta S_k^{(i)}, \quad (7)$$

where  $T_c$  is determined from the system of algebraic equations

$$\sum_{i=1}^m \sum_{k=1}^{N_i} \alpha_{ih} (T_h^{(i)} - T_c) \Delta S_k^{(i)} = 0, \quad (8)$$

and  $\alpha_{ih}$  are determined from the corresponding criterional relations [21, 22]. In the corresponding program module the heat-transfer coefficients are calculated, the system (8) is solved, and the resulting convective heat fluxes are determined for a fixed spatial partitioning and configuration of the cavity. The program modules which take into account the radiative and conductive heat transfer in narrow annular channels, and heat transfer under conditions of forced convection, fulfill analogous functions.

Modules of the third type are used to automate the separate stages of the transition from the parameters of real structures to the output data of the programs of the first and second types. These modules include, for example, programs which automatically construct the spatial grid for the transverse sections of noncanonically shaped elements. Index matrices, employed in the modules which implement the calculation of the temperature fields of these bodies using the method of finite elements, are formed in them.

In using the program complex described above to model the thermal regimes of quantrons the time-dependent and spatial distributions of the volume and surface heat sources are assumed to be given and enter into the starting data. The spatial distributions are calculated with the help of a special complex of programs, based on the use of the Monte Carlo method [23]. The time-dependent distributions are determined based on the procedure described in [24].

Computational Results. The complex was used to analyze the thermal regimes in designing quantrons with different constructions — with a hollow reflector, with a hollow reflector and the active element placed in a tube made of a material with a high thermal conductivity, with a single-block reflector, etc., using different active media (glass activated with neodymium, yttrium-aluminum garnet, gadolinium-scandium-gallium garnet, potassium-gadolinium tungstenate, etc.) — for different temporal operating states. Figure 2 shows as an example the temperature distribution in the middle section of the active element of two quantrons.

At the same time, based on the results of calculations of time-varying three-dimensional temperature fields of the elements in quantrons the decrease in the gain in the active medium, the thermo-optical distortions arising in the active element, the perturbations they introduce into the optical resonator and, finally, the changes in the output energy of the laser were determined [3].

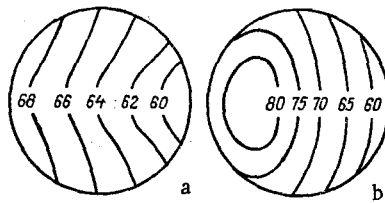


Fig. 2. Temperature field in the middle section of an yttrium-aluminum garnet active element in a quantron with a circular hollow reflector (a) and a potassium-gadolinium tungstenate garnet in a quantron with an elliptical hollow reflector (b). The flash-lamp is on the left. The lines show the isotherms and the numbers are the temperatures in °C.

Important characteristics of any program complex, intended for use in automated design systems, are the mean computing time and also the mean time required for the user in preparing the starting data for one variant of the calculation. Experience in using the program complex described showed that the average time required for calculating a nonstationary temperature field for a quantron with the typical construction with a numerical error of 4-5%, determined by Runge's rule [25], equals 5-10 min on the ES-1045 computer. Preparation of the starting data requires on the average 15 min. The comparatively small amount of engineering and computer time required for the calculation with the help of the program complex developed and the satisfactory agreement of the computational results with the experimental data [26] enable recommendation of the models developed, the numerical computational procedure, and the program complex for use at the computational stage in the design of solid-state lasers.

#### NOTATION

$\rho$ ,  $c$ , and  $\lambda$ , density, specific heat capacity, and thermal conductivity of the material of an element in the quantron or coolant;  $T$ , temperature field of an element in the quantron or coolant;  $\bar{x} = x, y, z$ , spatial coordinates;  $\tau$ , time coordinate;  $q_v$  and  $q_s$ , volume and surface heat flux density in elements of the quantron;  $T_0$ , starting temperature distribution in an element of the quantron or coolant;  $v_z$ , velocity of the coolant along the  $z$  axis;  $L$ , ratio of the perimeter of the cooling channel to its cross-sectional area;  $T_{in}$ , temperature of the coolant at the inlet to the cooling channel;  $n$  is the normal to the surface of the element;  $\Gamma$ , surface of the element;  $\alpha_k$ , heat-transfer coefficient between the elements of the quantron;  $\alpha$ , coefficient of heat transfer from an element of the quantron to the coolant or to the surrounding medium;  $\beta_r$ , a coefficient describing the heat transfer by radiation between the elements of the quantron;  $S$ , area of the surface of an element of the quantron;  $\sigma$ , Stefan-Boltzmann constant;  $\varphi$ , irradiance coefficient;  $m$ , number of elements in the quantron;  $l$ , total number of elements in the quantron and coolants;  $N$ , number of sections into which the surface of an element of the quantron is partitioned. Indices:  $i, v$ , number of an element of the quantron;  $j$ , number of an element in the coolant.

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NUMERICAL SOLUTION OF AN INVERSE PROBLEM IN NONSTATIONARY MASS TRANSFER  
IN A MULTICOMPONENT MIXTURE

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Discrepancy-functional minimization is used to show that there is considerable interaction between adsorbed components during transport in a porous material.

A major problem in the theory of heat and mass transfer concerns methods of solving inverse problems, which have been classified in [1-3]; one needs numerical values for the kinetic coefficients to simulate and optimize mass-transfer equipment. To determine these for mixtures, it is necessary to solve for kinetic-parameter matrices [4]. One measures the concentrations averaged over the volumes of the porous particles, which are dependent on run time (kinetic curves) when one examines nonstationary transfer in sorbents and catalysts. An inverse problem in mass transfer for a binary mixture can [5] be handled by determining the elements in the coefficient matrix by using sections of the kinetic curves. Here we consider a method of solving for nonstationary mass transfer for an n-component mixture, which is based on minimizing the discrepancy functional, where it is shown that there is a considerable interaction between the components within the material.

The mass flux densities are put as [6]

$$j = -D\nabla a. \quad (1)$$

We consider the simplest case of boundary conditions of the first kind. The equations for nonstationary mass transfer for an n-component mixture subject to constant values for the elements of matrix D may be written as

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