Journal of Engineering Physics and Thermophysics, Vol. 69, No. 2, 1996

MATHEMATICAL MODELING OF LASER-INDUCED DIFFUSION PROCESSES

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UDC 537.311.322.6:539.219.2

The possibility of using lasers to form semiconductor materials (cadmium and mercury tellurides) with a predetermined width of the band gap was explored using mathematical modeling. A one-dimensional physicomathematical model based on diffusion and heat conduction equations and transport equations for laser radiation with temperature- and concentration-dependent coefficients was used. Self-similar solutions were used in order to obtain certain qualitative regularities of the processes. In the general case the corresponding system of partial differential equations was integrated numerically.

Introduction. Semiconductor compounds of elements of the second and sixth groups of the periodic table play an important part in modern semiconductor physics and engineering, being most important and promising materials in a series of rapidly developing branches of science and technology, especially photo- and optoelectronics, quantum radiophysics, and acoustoelectronics. This is primarily connected with the fact that these compounds have various values of the band-gap width: from zero to several electron-volts, which makes it possible to vary their electric, photoelectric, and optical properties over a wide range. The conductivity of substances of this class can vary from values corresponding to a semimetal to those characteristic for an insulator, and the spectral zone of photosensitivity – from IR to UV.

In this connection interest is growing in investigating various physical properties of the compounds mentioned, in particular, narrow-band-gap semiconductors, which (especially solid $Cd_xHg_{1-x}Te$ solutions with $x = 0.2-0.3$) have been widely used in recent years as a material for fabricating photosensors operating in the ranges 3–5 and 8–14 μm. Photosensors fabricated from these compounds already dominate in IR imaging technology and lidar and communication systems.

Several methods of production of cadmium and mercury tellurides exist. The present work is devoted to mathematical modeling of laser-induced diffusion processes for production of semiconductor materials based on AB-type compounds with a predetermined width of the band gap ($Cd_xHg_{1-x}Te$ alloys). A one-dimensional physicomathematical model based on diffusion and heat conduction equations and transfer equations for the laser radiation with temperature- and concentration-dependent coefficients is employed. In order to investigate a series of qualitative regularities, self-similar solutions are considered. In the general case the analysis is carried out numerically.

The aim of the present work is to analyze the possibility of use of lasers to form semiconductor materials with a required width of the band gap in the system of an epitaxial film of a narrow-band-gap semiconductor and a substrate of a wide-band-gap AB-type semiconductor. The possible qualitative character of phenomena taking place in the course of this process is described, e.g., in [1]. Laser radiation with a wavelength corresponding to the width of the band gap of the material being produced passes through a transparent wide-band-gap semiconductor and is absorbed by a narrow-band-gap one. As a result, intense local heating takes place at the interface of the materials, which leads to acceleration of mutual diffusion and formation of a semiconductor alloy having a band gap of an intermediate width. Repeated laser action leads to motion of the zone of localized absorption toward the film-air interface and formation of an alloy of the required composition. The processes of mutual diffusion can be controlled by varying parameters of the laser radiation and the original materials.

Institute of Mathematical Simulation, Russian Academy of Sciences, Moscow. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 69, No. 2, pp. 194-205, March-April, 1996. Original article submitted June 26, 1995.

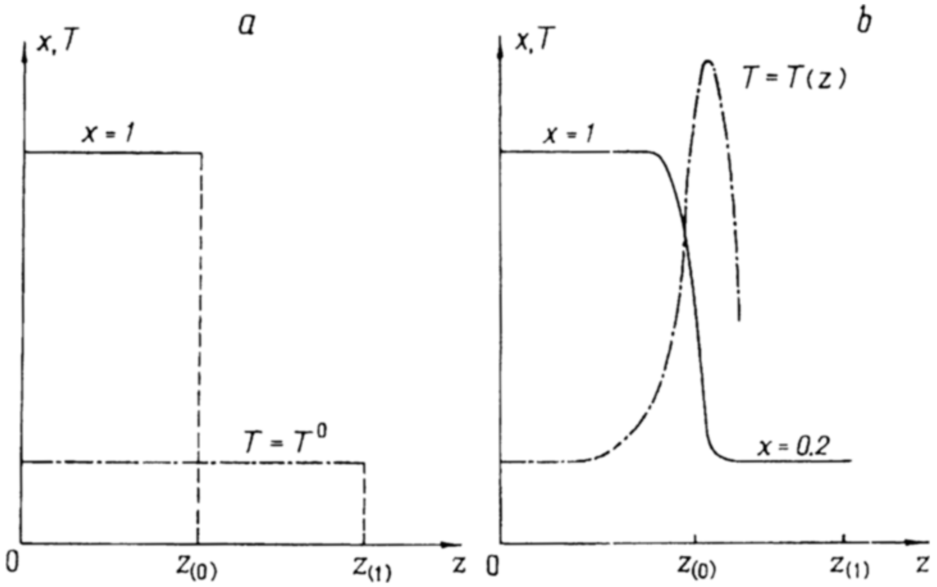


Fig. 1. Formation of temperature and concentration profiles for production of a semiconductor alloy.

Principles of the method developed to carry out numerical experiments are outlined in the monograth [2].

Particular calculations were carried out for semiconductor materials consisting of $Cd_{0.2}Hg_{0.8}Te$ alloys. The possibility of forming of a semiconductor consisting of $Cd_xHg_{1-x}Te$ alloy was estimated. In accordance with the width of the band gap of the material obtained, use of a laser with a wavelength $\lambda = 10.6$ μm was considered. It was assumed that the temperature of the system must not exceed the melting temperature of the investigated materials in the process of mutual diffusion and heat transfer.

1. Statement of the Problem. Basic Equations. Processes of mutual diffusion and heat transfer attributable to absorption of laser radiation and the mechanism of heat conduction that take place in $Cd_xHg_{1-x}Te$ alloys can be described by the following system of equations [3-7]:

$$\frac{\partial x}{\partial t} = - \operatorname{div} J , \tag{1.1}$$

$$\rho C \frac{\partial T}{\partial t} = - \operatorname{div} W - \operatorname{div} q , \tag{1.2}$$

$$J = - D \operatorname{grad} x , \tag{1.3}$$

$$W = - \kappa \operatorname{grad} T , \tag{1.4}$$

$$\operatorname{div} q = - kq . \tag{1.5}$$

The specific heat of the medium and the coefficients of mutual diffusion, thermal conductivity, and absorption of radiation are generally functions of concentration and temperature. Additional diffusional fluxes resulting from the temperature gradient (thermodiffusion) are not taken into account. We treat diffusion and heat transfer processes within the plane symmetry approximation. Then the sought functions will depend on the time t and the spatial coordinate z.

Let $z = 0$ be the coordinate characterizing the boundary of the system under consideration on which the flux of laser radiation with a time-dependent density $q(0, t) = Q(t)$ is predetermined. Under the assumptions specified the system of equations (1.1)-(1.5) can be written as follows:

$$\frac{\partial x}{\partial t} = \frac{\partial}{\partial z}\left(D \frac{\partial x}{\partial z}\right), \tag{1.6}$$

$$\rho C \frac{\partial T}{\partial t} = -\frac{\partial W}{\partial z} - \frac{\partial q}{\partial z}, \tag{1.7}$$

$$W = -\kappa \frac{\partial T}{\partial z}, \tag{1.8}$$

$$q = Q(t) \exp\left(-\int_0^{z_0} k dz'\right). \tag{1.9}$$

We will assume that at the initial instant $t = 0$ a substrate consisting of CdTe ($x = 1$) alloy with a density $\rho(z, 0) = \rho^0_{(1)}$ occupies the region $0 \le z \le z_{(0)}$ and a layer of HgTe ($x = 0$) with a density $\rho(z, 0) = \rho^0_{(0)}$ deposited on the substrate occupies the region $z_{(0)} \le z \le z_{(1)}$ (see Fig. 1a). The initial temperature is constant within the region $0 \le z \le z_{(1)}$: $T(z, 0) = T^0$. As was mentioned in the Introduction, at the initial instants, as a result of transparency of CdTe alloy, the radiation $Q(t)$ reaches the boundary $z = z_0$, where it is absorbed. The local heating resulting from this circumstance leads to mutual diffusion of particles and heat transfer due to thermal conductivity. The process lasts up to a certain instant $t = \bar{t}$ at which the local-heating zone (the zone of absorption of the laser radiation) reaches the right boundary of the system $z = z_{(1)}$. The objective of the investigation was an estimate of the possibilities of forming $Cd_{0.2}Hg_{0.8}Te$ semiconductor alloy by the time $t = \bar{t}$, i.e., the concentration profile $x = x(z, \bar{t})$ depicted in Fig. 1b ($x \simeq 0.2$ when $z_{(0)} \lesssim z \lesssim z_{(1)}$).

We consider the system (1.6)-(1.9) subject to the following boundary conditions. At the left boundary $z = 0$ the following conditions are set:

$$x(0, t) = 1, \quad T(0, t) = T_{(0)}, \quad q(0, t) = Q(t), \tag{1.10}$$

whereas at the right boundary $z = z_{(1)}$

$$\left.\frac{dx}{dz}\right|_{z=z_{(1)}} = 0, \quad T(z_{(1)}, t) = T_{(1)}. \tag{1.11}$$

We will assume that the alloys under investigation remain solid during the entire process, i.e., the temperature does not exceed the melting temperature T^*. This constraint imposed on the temperature is met by specifying discontinuous variations of the laser radiation with time at the boundary $z = 0$.

The flux density of the laser radiation within the interval $\tau_{2n} \le t \le \tau_{2n+1}$, $n = 0, 1, \ldots$ at the boundary $z = 0$ is assumed to vary linearly with time:

$$Q(t) = Q_0 (t - \tau_{2n}). \tag{1.12}$$

Absorption of radiation leads to an increase in the temperature. Upon reaching the value $T_{\max}(\tau_{2n+1}) \simeq T^*$ the laser pulse is shut off. Then for $\tau_{2n+1} \le t \le \tau_{2n+2}$, $n = 0, 1, \ldots$ we assume that $Q(t) = 0$, which leads to cooling of the system. The laser pulse at the boundary starts to act again when the temperature decreases to the value $T_{\max}(\tau_{2n+1}) = \chi T^0$, where $T^0 \le \chi T^0 \le T^*$, $\chi \ge 1$ being a constant parameter.

Computational experiments were carried out using the following numerical values of the parameters: $z_{(0)} = 7.6 \cdot 10^{-2}$ cm, $z_{(1)} = 7.8 \cdot 10^{-2}$ cm, $\rho^0_{(1)} = 8.084$ g/cm^3, and $\rho^0_{(0)} = 5.85$ g/cm^3.

It was assumed that $T_{(0)} = T_{(1)} = T^0$, and the values $T^0 = 300$ K and $T^0 = 77$ K were considered. The laser pulse was shut off when the temperature reached the value $T = 800$ K, close to the melting temperature of HgTe ($T^* = 848$ K), and was switched on again at $\chi T^0 = 400$ K. A laser with a wavelength of 10.6 μm (the corresponding photon energy $h\nu = 0.1$ eV) was considered. The constant Q_0 in Eq. (1.12) was varied, but it was assumed that in each variant its value is the same for all laser pulses.

It is shown in [8] that the concentration dependence of the density can be approximated by a linear dependence. In view of the preset values of $\rho^0_{(1)}$ and $\rho^0_{(0)}$ we obtain

$$\rho(x) = (5.85 + 2.234x) \quad \text{g/cm}^3 .$$

2. Transfer Coefficients. Specific Heat. Unfortunately, complete information on the coefficients of absorption and thermal conductivity and the specific heat for alloys of the type $Cd_xHg_{1-x}Te$ within the ranges of variation of concentration x and temperature T of interest is lacking at the present time. In the present work the corresponding expressions are obtained by means of extrapolation of existing experimental and numerical data presented in [8-12].

The absorption coefficient was calculated by the following expressions:

$$k = \begin{cases} 10^{3.45-3.214x} & \text{when} \quad 0 \le x \le 0.14 , \\ 10^{5.1-15x} & \text{when} \quad x \ge 0.14 . \end{cases} \tag{2.1}$$

The absorption coefficient is assumed to be temperature-independent within the calculation region 77 K $\le T \le$ 800 K.

The dependence of the thermal-conductivity coefficient on temperature and concentration was specified by a table based on data presented in [8]:

$$\kappa(x, T) = \kappa_{\text{table}} = \kappa_{k,l}, \quad \log \kappa_{k,l} = f(\log x_k, \log T_l) ,$$

where $10^{-4} \le x_k \le 1$, 77 K $\le T \le$ 900 K. Within the intervals $x_k \le x \le x_{k+1}$ and $T_l \le T \le T_{l+1}$ the function log κ is determined by linear interpolation from points log $\kappa_{k,l}$ defined by the table.

The specific heat $C = C(x, T)$ is determined by a formula presented in [8, 13] for CdTe alloy:

$$C = (11.79 + 2.06 \cdot 10^{-3}\, T) \quad \text{cal} \cdot \text{mole}^{-1} \cdot \text{K}^{-1} . \tag{2.2}$$

The mutual-diffusion coefficient is calculated by a formula used for regular solid alloys under the assumption that the temperature and the pressure are constant (see, e.g., [3, 14, 15]). For the mixture under consideration this formula can be written as follows:

$$D = [D_1 (1 - x) + D_2 x]\, g , \tag{2.3}$$

where the function

$$D_1 = D_{10} \exp(-E_1/(kT)) \tag{2.4}$$

is the self-diffusion coefficient of Cd in Hg, and the function

$$D_2 = D_{20} \exp(-E_2/(kT)) \tag{2.5}$$

is the self-diffusion coefficient of Hg in Cd. In expressions (2.4) and (2.5) D_{10} and D_{20} are constant factors, k being the Boltzmann constant. The parameters E_1 and E_2 determine the corresponding activation energy of each of the components of the alloy under consideration and are assumed to be constant.

The factor g entering the expression (2.3) characterizes the deviation from ideal alloys due to the mixing (ordering) energy – the deviation caused by interaction of each atom of the crystal lattice with atoms situated within the closest coordination sphere. The function g is represented as follows:

$$g = 1 + 2lE_{\text{mix}}\, x(1 - x)/(kT) ,$$

where E_{mix} is the mixing energy and l is the coordination number determined by the lattice structure. The aforementioned constants were assumed to take the following values: $D_{10} = 1374\ \text{cm}^3/\text{sec}$, $D_{20} = 1.1 \cdot 10^{-5}\ \text{cm}^2/\text{sec}$, $E_1 = 2.61$ eV, $E_2 = 0.58$ eV, and $l = 8$.

It follows from the preceding that the expressions for the transfer coefficients and specific heat used in the calculations are very approximate. In order to determine the qualitative character of the influence of each of the aforementioned factors on the mutual diffusion and heat transfer in computational experiments we varied the corresponding "material constants."

In order to investigate certain qualitative regularities of the processes under investigation we consider below self-similar solutions obtained under simplifying conditions. Methods of solution of problems of this type are given, for example, in [16].

3. **Self-Similar Problem.** Instead of the original system of equation, we consider equation describing diffusion and heat transfer processes in a medium with a constant density, thermal conductivity, and specific heat. In addition we will assume that the absorption coefficient is a power function of the coordinate and the time, and the source of the laser radiation is described by a power function of the time:

$$k = k_0 t^{\alpha} z^{\beta}, \quad q(0, t) = q_0 t^{g}. \tag{3.1}$$

Neglecting terms that are small when $0 < x \le 1$ in the expression for the diffusion coefficient, one can represent (2.3) in the following form:

$$D = D_0 x \left[1 + 2x(1 - x) \frac{A_1}{T} \exp(-l/T) \right], \tag{3.2}$$

where $D_0 = D_{20}$; $A_1 = 2zE_{\text{mix}}/K$; $l = E_1/K$. The boundary conditions are set as follows:

$$x(0) = 1, \quad x(\infty) = 0{,}2, \quad J(\infty) = 0, \quad T(0) = T(\infty) = T_0. \tag{3.3}$$

In view of the above assumptions the system (1.6)-(1.9) takes the form

$$\frac{\partial x}{\partial t} = -\frac{\partial J}{\partial z}, \tag{3.4}$$

$$J = -D \frac{\partial x}{\partial z}, \tag{3.5}$$

$$\frac{\partial T}{\partial t} = \frac{\kappa_0}{\rho_0 C_0} \frac{\partial^2 T}{\partial z^2} + \frac{k q_0}{\rho_0 C_0} t^{\zeta}, \tag{3.6}$$

$$\frac{\partial q}{\partial z} = -kq, \tag{3.7}$$

$$k = k_0 t^{\alpha} z^{\beta}. \tag{3.8}$$

Dimensional analysis leads to the following self-similarity conditions for the problem (3.1)-(3.8):

$$\zeta = -1/2, \quad \beta + 2\alpha = -1. \tag{3.9}$$

Due to self-similarity the sought functions will depend on a dimensionless combination of the form $s = z/(M_0 t^{0.5})$, where M_0 is a constant expressed in terms of the parameters $\kappa_0/(\rho_0 C_0)$ and T_0. In this case the sought functions can be represented in the form

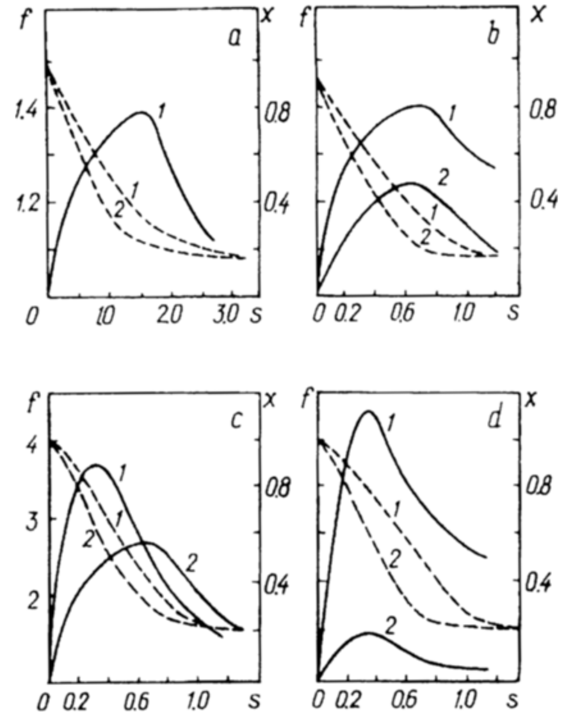


Fig. 2. Dependence of dimensionless functions of temperature $f = f(s)$ (solid lines) and concentration $x = x(s)$ (dashed lines) in the case where one of the constant parameters is varied and the others are fixed: a) mixing energy A_1: 1) $A_1 = 10$; 2) $A_1 = 2$; b) absorption coefficient $\hat{k}_0$: 1) $\hat{k}_0 = 2$; 2) $\hat{k}_0 = 1$; c) of thermal-conductivity coefficient $\hat{\kappa}_1$: 1) $\hat{\kappa}_1 = 0.01$; 2) $\hat{\kappa}_1 = 0.1$; d) power of the laser source $\hat{q}_1$: 1) $\hat{q}_1 = 10$; 2) $\hat{q}_1 = 1$.

$$x(s) = x(z, t), \quad T(z, t) = T_0 f(s), \quad J(z, t) = \hat{J}(s)\, M_0/t^{0.5},$$

$$W(z, t) = w(s)\, T_0/(M_0 t^{0.5}). \tag{3.10}$$

Using the substitution of variables (3.10) in the system (3.4)-(3.8), we obtain the following system of ordinary differential equations

$$-0.5s \frac{df}{ds} = -\hat{\kappa}_1 \frac{dw}{ds} + \hat{k}_0 \hat{q}_1 s \exp(-\hat{k}_0 s^2/2), \tag{3.11}$$

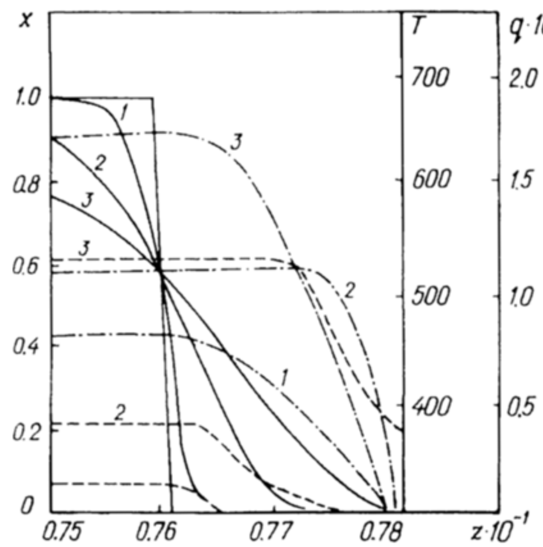
$$w(s) = -\frac{df}{ds}, \tag{3.12}$$

$$0.5s \frac{dx}{ds} = \frac{d\hat{J}}{ds}, \tag{3.13}$$

$$\hat{c}_1 = A_1/f(s), \quad \hat{c}_2 = \exp(-l/f(s)). \tag{3.14}$$

$$\hat{J} = -\hat{D}_0 x\, [1 + 2x(1 - x)\, \hat{c}_1]\, \hat{c}_2 \frac{dx}{ds}, \tag{3.15}$$

where $\hat{\kappa} = \kappa_0/(\rho_0 C_0)$, $\hat{k}_0 = k_0$, $\hat{q}_1 = q_0 \rho_0^{-1} C_0^{-1}$, and $\hat{D}_0 = D_0$ are dimensionless constants.



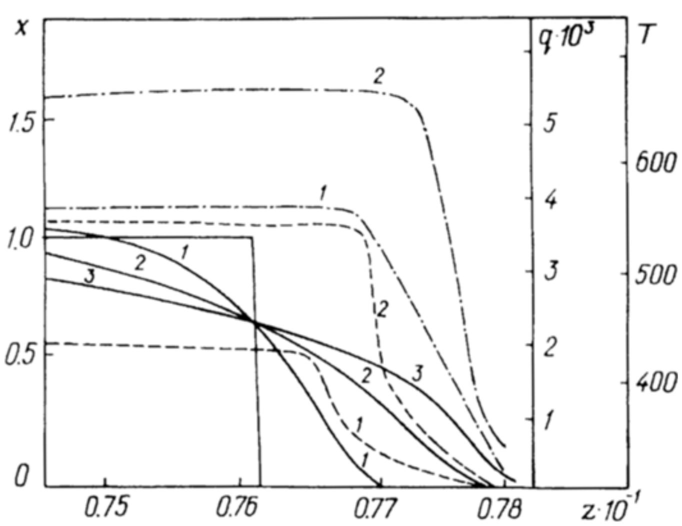


Fig. 3. Distributions of the concentration x (solid lines), temperature T (dash-dot lines), and flux density of the radiation q (dashed lines) over the spatial coordinate z for various instants of time: 1) $t = 9.95\cdot 10^2$ sec; 2) $1.985\cdot 10^3$ sec; 3) $1.238\cdot 10^4$ sec, for $\kappa = \kappa_{\text{table}}$, $A_1 = 0$, $T_0 = T_1 = 300$ K, $Q_0 = 2$.

Fig. 4. Profiles analogous to those presented in Fig. 3 for $Q_0 = 2000$ at the instants $t = 2\cdot 10^1$ sec (1), $9.96\cdot 10^2$ sec (2) and $3.497\cdot 10^3$ sec (3).

The initial and boundary conditions (3.3) written in the new variables take the form

$$f(0) = f_0 ,\quad f(\infty) = f_0 ,\quad x(0) = 1 ,\quad x(\infty) = 0{,}2 ,\quad J(\infty) = 0 . \tag{3.16}$$

The system of heat conduction equations (3.11), (3.12) admits the analytical solution

$$f(s) = f_0 + 2\hat{q}_1 \sqrt{(2\hat{k}_0)}\, [\operatorname{erf}(\sqrt{(0.5\hat{k}_0)}\, s) - \operatorname{erf}(s/(2\sqrt{(\hat{\kappa}_1)}))]/(2\hat{k}_0 \hat{\kappa} - 1) , \tag{3.17}$$

$$w(s) = -\frac{\hat{q}_1 \sqrt{\hat{k}_0}}{2\hat{k}_0 \hat{\kappa}_1 - 1} \sqrt{\left(\frac{2}{\hat{\kappa}_1}\right)} \exp(-0.5\hat{k}_0 s^2)\, [\sqrt{(2\hat{k}_0 \hat{\kappa}_1)} - \exp(4\hat{\kappa}_1 s^2 (2\hat{k}_0 \hat{\kappa}_1 - 1))] . \tag{3.18}$$

The system of diffusion equations (3.13)-(3.15) must be integrated numerically. In order to determine a direction of stable integration for the system of equations (3.13)-(3.15) we consider its asymptotic solutions in the vicinity of $s = \infty$ and $s = 0$. Let $x(0) = x_2 = 1$, $x(\infty) = x_1 = 0.2$, and $I(\infty) = 0$. When $s \to \infty$ we obtain $\hat{c}_1 \to c_1$, $\hat{c}_2 \to c_2$, where c_1 and c_2 are constants. The system (3.13)-(3.15) can be written in the following form with accuracy up to the dominant terms:

$$0.5s \frac{dx}{ds} = \frac{d\hat{J}}{ds} , \tag{3.19}$$

$$\hat{J} = -D_1 \frac{dx}{ds} + \dots , \tag{3.20}$$

where $D_1 = \hat{D}_0 x_1 (1 + 2x_1(1 - x_1)c_1)$, and c_2 is a constant.

The solution of the system (3.19)-(3.20) is as follows:

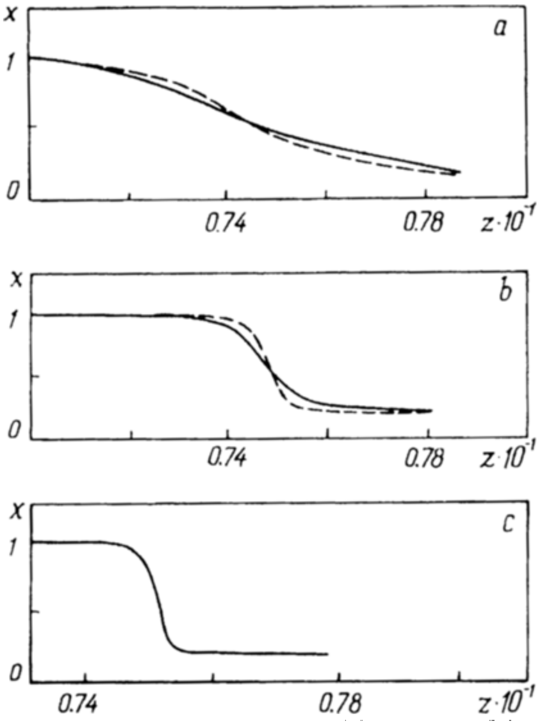


Fig. 5. Profiles of the function $x = x(z)$ at the instants $t = \bar{t}$ for various values of the parameter κ, mixing energy A_1, and radiation power Q_0: a) $\kappa = \kappa_{\text{table}}$, $A_1 = 2.4 \cdot 10^5$ for $Q_2 = 2$ at $t = 7.09 \cdot 10^2$ sec (solid line) and $Q_0 = 20$ at $\bar{t} = 1.075 \cdot 10^3$ sec (dashed line); b) analogous profiles for $\kappa = \kappa_{\text{table}} \cdot 10^{-7}$ and $A_1 = 2.4 \cdot 10^5$; c) $\kappa = \kappa_{\text{table}} \cdot 10^{-7}$, $A_1 = 2.4 \cdot 10^7$, $Q_0 = 20$, $t = 90.92$ sec.

$$\hat{J} = c \exp\left(-s^2/(4D_1)\right) + \dots, \tag{3.21}$$

$$x(s) = -\frac{2c}{\sqrt{D_1}} \operatorname{erf}\left(s/2\sqrt{D_1}\right) + c_3 + \dots, \tag{3.22}$$

with the following relationship between the constants being satisfied:

$$-c\sqrt{\left(\frac{\pi}{D_1}\right)} + c_3 = x_1 .$$

It follows from (3.21) that the integral curves approach each other arbitrarily closely, and therefore integration in the direction from the point $s = \infty$ to the point $s = 0$ is impossible due to rounding-off errors.

Let us consider the behavior of the integral curves in the vicinity of the point $s = 0$. When $s \to 0$, we obtain $x \to x_2 = 1$, $\hat{c}_2 \to c_2$ (c_2 is a constant). The system of diffusion equations (3.13)-(3.15) is as follows with accuracy up to the dominant terms:

$$0.5s \frac{dx}{ds} = \frac{d\hat{J}}{ds}, \tag{3.23}$$

$$\hat{J} = -D_2 \frac{dx}{ds} + \dots, \tag{3.24}$$

where $D_2 = \hat{c}_2 D_0$.

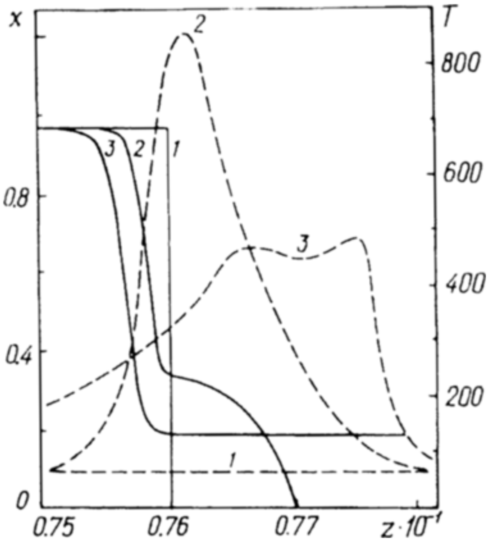


Fig. 6. Dynamics of processes for the variant presented in Fig. 5c: $x = x(z)$ (solid line) and $T = T(z)$ (dashed line) for $t = 0$ (1), 16.46 sec (2), and 90.92 sec (3).

The equations (3.23), (3.24) are analogous to the equations (3.19), (3.20), which describe the asymptote when $s \to \infty$. Therefore the solution is written in an analogous manner:

$$\hat{J} = c_4 \exp\left(-s^2/(4D_2)\right) + \ldots, \tag{3.25}$$

$$x(s) = -\frac{2c_4}{\sqrt{D_2}} \operatorname{erf}\left(\frac{s}{2\sqrt{D_2}}\right) + c_5 + \ldots \tag{3.26}$$

The condition $x(0) = 1$ yields $c_5 = 1$.

It is evident from the expressions for the flow (3.21), (3.25) that integration from the point $s = 0$ to the point $s = \infty$ is stable.

The overdetermination of the system is removed in this case by finding the constant $c_4 = \hat{J}(0)$ by means of adjustment.

Figure 2 presents results of calculations in which one of the constant parameters was varied, and the values of the others were kept unchanged. It is evident from the figure that an increase in the parameters A_1, $\hat{k}_0$, i.e., the mixing energy and the absorption coefficient, leads qualitatively to the same results as an the increase in the thermal-conductivity coefficient and the power of the laser source $\hat{\kappa}_1$ and $\hat{q}_1$. The calculations also showed that a decrease in the value of the specific heat C_0 qualitatively affects the behavior of the solution analogously to an increase in the parameter of the mixing energy A_1.

4. Results of Computational Experiments. The system of equations (1.6)-(1.9) with corresponding boundary conditions was solved by the finite-difference method using the integro-interpolational method for constructing difference schemes [2]. An implicit difference scheme was considered that was solved by the well-known sweep method.

1. The first series of computational experiments was carried out using the expressions for the coefficients of the original equations (1.6)-(1.9) that were presented in the Sec. 2 of the present paper, including the case where $\kappa = \kappa_{\text{table}}$ and the diffusion coefficient is of the form (2.3) with $g \equiv 1$, i.e., assuming that the alloys are ideal. The initial and, correspondingly, boundary values of the temperature were taken to be equal to the value $T^0 = 300$ K. In different variants of the calculations we varied the parameter Q_0 that enters the formula (1.12), i.e., the rate of increase of the flux density of the first and all succeeding pulses. The main results of the calculations are presented in Figs. 3 and 4.

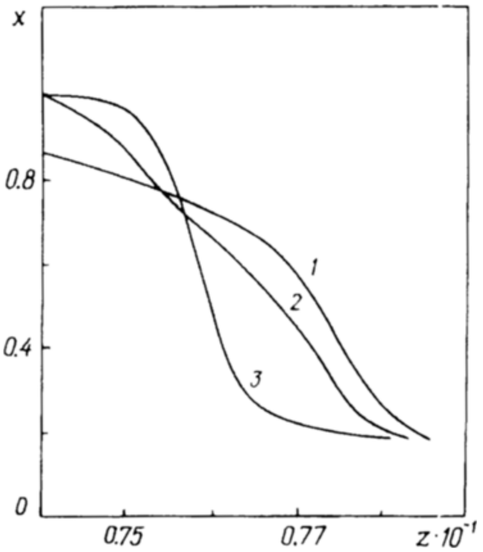


Fig. 7. Profiles of $x = x(z)$ for $\kappa = \kappa_{\text{table}}$, $A_1 = 2.4\cdot 10^7$ for various values of the specific heat C: 1) $C = C_{(2.2)}$ (i.e., the specific heat calculated by the formula (2.2)) at the instant $\bar{t} = 3.798$ sec; 2) $C = C_{(2.2)}\cdot 10^2$ at $\bar{t} = 43.4$ sec; 3) $C = C_{(2.2)}\cdot 10^7$ at $\bar{t} = 1.75\cdot 10^3$ sec.

It follows from the calculations that an alloy of the required composition cannot be produced under the assumptions indicated above. In this case the qualitative character of the spatial distribution of the sought quantities is conserved with change in the parameter Q_0. An increase in the value of the parameter Q_0 just leads to a decrease in the time interval $t = \bar{t}$ in which the zone of absorption of the laser radiation (the zone of local heating) reaches the outer boundary of the system $z = z_{(1)}$. In the case $Q_0 = 2$ we obtain $\bar{t} = 1.238\cdot 10^4$ sec, and for $Q_0 = 2\cdot 10^3$ we obtain $\bar{t} = 3.497\cdot 10^4$ sec. With increasing values of Q_0 the number of "switching-offs" of the laser pulse at moments when the temperature maximum reaches a value close to the melting temperature of the alloy also increases.

2. The next series of calculations was carried out taking into account the effect of the mixing energy on the mutual diffusion of alloys. In the variants indicated the value of the thermal conductivity coefficient κ was also varied (see Figs. 5 and 6).

In the variant corresponding to Fig. 5c we obtain the required profile $x = x(z)$: $x \simeq 0.2$ within the region $760\,\mu\text{m} \le z \le 780\,\mu\text{m}$. The dynamics of the process of mutual diffusion and heat transfer in this case in the time interval $0 \le t \le \bar{t} = 90.92$ sec is illustrated by the curves in Fig. 6.

We should also note that in the latter variant of the calculations the laser pulse was cut off a considerable number of times. In this case the time of action of each pulse that leads to an increase in the temperature maximum to values close to the melting temperature ($T = 800$ K) was of the order of $(1-3)\cdot 10^{-2}$ sec. The characteristic time of cooling to temperature values $T \simeq 400$ K after the end of the action of a laser pulse was equal to approximately 10 sec.

3. The third group of calculations was carried out for the values of the parameters $\kappa = \kappa_{\text{table}}$, $A = 1.2\cdot 10^7$ K and various values of the specific heat C (see Fig. 7). It is evident that the concentration profile $x = x(z)$ approaches the required one with increase in C.

The computational experiments carried out demonstrate that the required composition of $\text{Cd}_{0.2}\text{Hg}_{0.8}\text{Te}$ alloy with a width of $\sim 20\,\mu\text{m}$ can be obtained either in the case of strong underestimation of the thermal-conductivity coefficient (see Figs. 5c and 6) or at rather high values of the specific heat (Fig. 7). Here in both cases we considered the expression for the mutual-diffusion coefficient (2.3) taking into account substantial deviations from the conditions of ideal alloys. This suggests that in order to provide an accurate description of the processes under investigation, a detailed analysis, both theoretical and experimental, of parameters of the materials under consideration is required. Due to the presence of considerable temperature gradients the formula expressing the self-diffusion coefficient requires substantial refinement.

In the calculations carried out the shape of the laser pulse was fixed. The problem of the effect of parameters of the laser pulse invites further investigation. An analysis of the processes under investigation in the case where melting is taken into account is also of considerable interest.

NOTATION

x, dimensionless concentration of Cd particles; z, spatial coordinate; t, time; ρ, density; T, temperature; W, heat flux density due to the thermal conductivity; $C = C(x, T)$, specific heat of the medium; $D = D(x, T)$, mutual-diffusion coefficient; $\kappa = \kappa(x, T)$, thermal-conductivity coefficient; $k = k(x, T)$, coefficient of absorption of the laser radiation; q, flux density of the laser radiation; $q(0, t) = Q(t)$, flux density of the laser radiation predetermined at the boundary $z = 0$; Q_0, power of the laser radiation; A_1, parameter proportional to the mixing energy (ordering energy) E_{mix}; $\hat{k}_0$, $\hat{\kappa}_1$, dimensionless values of the absorption and thermal-conductivity coefficients in the self-similar solution.

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