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A theoretical model of temperature dynamics of the solid surface of a material under action of laser radiation

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Abstract. We have developed a theoretical model that describes the interaction of intense pulsed flows of energy with matter and is based on the account of local phase transitions at the destruction of a surface. In the frame of a problem concerning the influence of a laser radiation on the surface prior to the beginning of the solid surface destruction, we have solved the equation for the energy flow. The general solution of the equation for the temperature change of a local area of the irradiated solid surface in time is obtained with regard for the coefficient of surface dissipative losses and the volume absorption coefficient. It is shown that the temperature dynamics stimulated by the intense laser radiation depends substantially on properties of the surface layer of the irradiated material.

Keywords: intensity of radiation, dissipative losses, volumetric absorption, hydrodynamic model of continuum, temperature dynamics, local changes..

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1. Introduction

Last years, the growing interest is paid to the use of very short and powerful laser pulses in the research of properties of materials [1-5]. Under the action of such pulses, the matter surface can collapse. The structure and properties of the superficial layer of a material (smoothness or roughness of the surface [2], porosity [3], absorptive ability, structure, physical and chemical properties) influences substantially the formation of the arising plasma torch.

In this connection, the development of a general theoretical approach to the processes which accompany the irradiation of the material surface by a laser in the pulsed mode will give possibility to forecast the consequences of this influence on surfaces of different types. The analysis of the $P - T$ diagram of the state of a material shows [5] that its "behavior" in the extreme state is determined by pressure and temperature [6]. In the analysis of the process of destruction, the hydrodynamic model of continuous environment is often used [4, 7].

2. General statement of a problem

The problems of the destructive or non-destructive effects of radiation on a surface are traditionally examined as different. But, if one considers that the

bordering phases which arise up at the destruction are continuous, the initial system of equations for them looks as follows [8]:

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{v}) = R_m \quad (1)$$

$$\frac{\partial v^i}{\partial t} + (\mathbf{v} \cdot \nabla) v^i - \frac{1}{\rho} \frac{\partial P_{ij}}{\partial x_j} = f^i, \quad (2)$$

$$\rho \frac{\partial U}{\partial t} + \rho (\mathbf{v} \cdot \nabla) U + \text{div} \mathbf{Q} = P_{ij} v_{ij}. \quad (3)$$

Here, U , ρ , \mathbf{v} are, respectively, the intrinsic energy of a mass unit of the continuous medium, density of this medium, and a convection velocity vector, \mathbf{Q} is the general energy flow in the medium, P_{ij} is the mechanical stress tensor, R_m is the function representing mass sources-outflows, \vec{f} is the mass force density, and $v_{ij} = \partial v^i / \partial x_j$ is the deformation velocity tensor, $\{i, j\} = \{1, 2, 3\}$.

If system (1)-(3) is examined for the gas phase, it is heterogeneous because of the presence of volume sources and flows, which arise up in the solid-gas phase transition, i.e. in the process of destruction [9]. When the destruction takes place, simultaneously there are the gas and solid phases. In this case, the stress tensor in the gas

volume $P_{ij} = -P\delta_{ij}$ [10]. From (1)-(3), it is possible at once to get a system of equations of the gas dynamics [11].

For the solid state of a material, the density is constant, and the functions $R_m = 0$. System (1)-(3) with regard for Hooke's laws can be written as [8]

$$\mathbf{v}_0 = 0. \quad (4)$$

$$\rho_0 \ddot{\mathbf{u}}_0 = \rho_0 \mathbf{f}_0 + (\nu + \mu) \nabla \operatorname{div} \mathbf{u}_0 + \mu \Delta \mathbf{u}_0, \quad (5)$$

$$\rho_0 \frac{dU_0}{dt} + \operatorname{div}(\mathbf{Q}_0) - P_{ij}^{(0)} v_{ij}^{(0)} = 0, \quad (6)$$

where \mathbf{u}_0 is the displacement vector, \mathbf{f}_0 is the mass density of a volume force, and ν and μ are the elastic constants. The displacement vector \mathbf{u}_0 and the velocity \mathbf{v}_0 are related by $\mathbf{v}_0 = d\mathbf{u}_0/dt$, where ρ_0 is the density of a condensed material, U_0 is the internal energy per unit mass of a solid substance, P_{ij} is the stress tensor, and \mathbf{Q}_0 is the energy flow penetrated into the volume of the solid medium.

For temperatures lower than the phase transition temperature, the internal energy can be written as $U_0 = -\varphi_0 + C_v^{(0)} T_0$. Using this relation and the definition of the energy flow $\mathbf{Q}_0 = \mathbf{q}_0 - \lambda_0 \cdot \operatorname{grad} T_0$ (it will be discussed below in more details) and neglecting the component $P_{ij}^{(0)} v_{ij}^{(0)}$ in (6), the energy equation reduces to the heat equation:

$$\rho_0 C_v^{(0)} \frac{\partial T_0}{\partial t} = \operatorname{div}(\lambda_0 \operatorname{grad} T_0) - \operatorname{div} \mathbf{q}_0, \quad (7)$$

where $\mathbf{q}_0(t, \mathbf{r})$ is the energy flow external with respect to the substance which acts in the solid phase volume; λ_0 is the heat conductivity coefficient; $T_0(t, \mathbf{r})$ is the surface temperature; and $C_v^{(0)}$ is the mass specific heat. In (7), we take into account both facts that the specific heat of the phase transition $\varphi_0 = \text{const}$ and $\frac{dT_0}{dt} = \frac{\partial T_0}{\partial t}$, inasmuch as the convective speed is absent in the solid phase.

3. Generalized boundary conditions for the problem of irradiation of a solid substance by a powerful pulse of radiation

System (1)-(3) is the initial system of differential equations. These equations describe simultaneously both phases, the solid and a gas. System (1)-(3) defines the behavior of a substance in the extreme state and unites two separate problems: with destruction and without it. For this system, it is necessary to formulate the boundary conditions on the interface of two phases.

The first boundary condition – the balance of mass flows across the boundary – can be obtained using the continuity equation [11]:

$$\rho_s (\mathbf{v}_s \cdot \mathbf{n}) - \rho_{0s} (\mathbf{v}_{0s} \cdot \mathbf{n}) = 0. \quad (8)$$

Here, ρ_s, \mathbf{v}_s are the superficial values of density and convective speeds in a gas phase, and $\rho_{0s}, \mathbf{v}_{0s}$ are the density and the velocity of “leakage” of the solid medium onto the phase interface. If the surface solid substance surface does not collapse under the action of radiation, the gas characteristics in Eq. (8) are absent:

$$(\mathbf{v}_{0s} \cdot \mathbf{n}) = 0. \quad (9)$$

The following condition of the balance of momentum flows is determined by analogy [8] on the basis of the second equation of system (1)-(3):

$$\rho_s v_s^i (\mathbf{n} \cdot \mathbf{v}_s) - P_{ij}^s n_j - \rho_{0s} v_{0s}^i (\mathbf{n} \cdot \mathbf{v}_{0s}) + P_{ij}^{(0)s} n_j = 0. \quad (10)$$

Here, $P_{ij}^s, P_{ij}^{(0)s}$ are the surface values of the stress tensor in the gas and solid phases, v_s^i, v_{0s}^i are, respectively, the i -th components of the vectors of speed of the gas and the condensed medium on their interface.

It is possible to present the stress tensor for the gas phase infinitely close to the surface as

$$P_{ij}^s = -P_s \delta_{ij} - \frac{1}{c} (\mathbf{n} \cdot \mathbf{q}_s) n_i. \text{ Here, the first component}$$

describes the elastic part of the stress tensor for gases [10], and the second component corresponds to the complementary light pressure on the solid surface. Thus, (10) takes the form

$$P_s n_i + \frac{1}{c} (\mathbf{n} \cdot \mathbf{q}_s) n_i + \rho_s (\mathbf{n} \cdot \mathbf{v}_s) (v_s^i - v_{0s}^i) + P_{ij}^{(0)s} n_j = 0. \quad (11)$$

Here, c is the light velocity, \mathbf{q}_s is an external radiation flow, and δ_{ij} is the Kronecker delta. If the destruction of a surface does not occur under the action of radiation, condition (11) becomes simpler because all components related to the destruction are absent. Then it is characterizes the elastic response of the condensed matter to the mechanically applied shock of the flow \mathbf{q} :

$$\frac{1}{c} (\mathbf{n} \cdot \mathbf{q}_s) n_i + P_{ij}^{(0)s} n_j = 0. \quad (12)$$

This relation is the boundary condition for Eq. (5), as well as for the processes running in the elastic medium, in particular for the transmission of sound and shock waves and for the elastic failure of the material, if it arises at energies less than the thermal one considered here.

The condition of balance of the energy flows follows from the system of equations (1)-(3) with the use of the equation for energy:

$$\begin{aligned} & \left(\mathbf{n} \cdot \mathbf{v}_s \right) \left(\rho_s U_s + \rho_s \sum_i \frac{(v_s^i - v_{0s}^i)^2}{2} - \rho_s U_{0s} + \left(1 - \frac{\rho_s}{\rho_{0s}} \right) P_s \right) + \\ & + \left(1 - \frac{\rho_s}{\rho_{0s}} \right) \frac{(\mathbf{n} \cdot \mathbf{v}_s)}{c} (\mathbf{n} \cdot \mathbf{q}_s) + (\mathbf{n} \cdot \mathbf{Q}_s) - (\mathbf{n} \cdot \mathbf{Q}_{0s}) = 0. \end{aligned} \quad (13)$$

The quantities $\mathbf{Q}_s = \mathbf{q}_s + \mathbf{q}_s^T$ and $\mathbf{Q}_{0s} = \mathbf{q}_{0s} + \mathbf{q}_{0s}^T$ are the general energy flows including the external (light) flow and the thermal flow. Here, \mathbf{q}_s is a part of the luminous flow which attains the surface; \mathbf{q}_{0s} is the surface flow which has transited into the condensed material; $-\lambda_{0s} (\text{grad } T_0)_s \equiv \mathbf{q}_{0s}^T$ and $-\lambda_s (\text{grad } T)_s \equiv \mathbf{q}_s^T$ are the superficial part of a thermal flow, respectively, in the solid and gas media.

In a case where no destruction of the surface happens, i.e. all the gas characteristics are absent, only two last components in Eq. (13) remain. Thus, in the environment, the flow \mathbf{q}_s^T is very small due to the smallness of both the temperatures gradient and the coefficient of heat conductivity [12] or exactly equals zero if the solid phase borders with vacuum. In the zone of contact of two phases, there occurs the formation of a surface layer, which is accompanied by the adsorption and the appearance of the surface energy, surface tension, surface electrical potential, and other specific surface properties. The surface layers are nonuniform on the scale of tens-hundreds of angstroms and differ from volumetric layers by their physical properties (density, viscosity, polarizability, etc.), a molecular structure, and a chemical composition (in multicomponent systems). In the surface layers, there can be such chemical effects as the deviation from the state of chemical equilibrium, change in the chemical reaction rates, and even a change in valence (for example, in valence of Sm, Cr). For this reason, it is necessary to account for losses of radiation at its passage through the surface layer of a substance. They can be characterized by the coefficient of dissipative losses L_d ($0 \leq L_d \leq 1$).

Respectively, a flow penetrating into the solid medium \mathbf{q}_{0s} and a flow which reaches a surface \mathbf{q}_s can be connected by the relation

$$\mathbf{q}_{0s} = (1 - L_d) \mathbf{q}_s. \quad (14)$$

Thus, the general relation of the energy balance of flows at the boundary for the nondestructive problem takes the form:

$$L_d (\mathbf{n} \cdot \mathbf{q}_s) + \lambda_{0s} (\mathbf{n} \cdot \text{grad } T_0)_s = 0. \quad (15)$$

This relation is the boundary condition for Eq. (7).

4. Change of the surface temperature under laser pulse action

We consider a spatially one-dimensional problem without dealing with the transverse shape of a pulse. Let

$\mathbf{q}_0 = \mathbf{e}_z q_0 \mathcal{G}(\tau - t)$ be the flow passed into the middle of a substance, where $\mathcal{G}(\tau - t)$ is the Heaviside function. We suppose that the heat conductivity coefficient λ_0 is a constant. The case where the thermal conductivity depends on T_0 has been considered in [13].

The magnitude of a volume flow q_0 inside the solid substance is determined by its amplitude value q_{0s} . Using (14), it is possible to write

$\mathbf{q}_0 = \mathbf{e}_z q_{0s} f(z) = \mathbf{e}_z (1 - L_d) q_s f(z) \equiv \mathbf{e}_z (1 - L_d) q$, where $q \equiv q_s f(z)$. Now the flow in the solid phase volume is specified by the peak value of an input flow.

Then the heat equation (7) takes the form

$$\rho_0 C_v^{(0)} \frac{\partial T_0}{\partial t} = \lambda_0 \frac{\partial^2 T_0}{\partial z^2} - \mathcal{G}(\tau - t) (1 - L_d) \frac{\partial q}{\partial z}. \quad (16)$$

Corresponding to this equation, the boundary condition [see (15)] is as follows:

$$\frac{\partial T_0}{\partial z}(t, 0) = -\frac{L_d}{\lambda_0} q_s \mathcal{G}(\tau - t). \quad (17)$$

Moreover, the boundary and initial conditions

$$T_0(0, z) = T_{in}, \quad T_0(t, \infty) = T_{in}$$

are valid, where T_{in} is the temperature of a material prior to the beginning of the radiation action.

The boundary condition (17) together with Eq. (16) consider, due to presence of the factor L_d , all possible losses at the interaction of radiation with the surface. This problem has two limiting cases: 1) losses at the substance surface under the energy flow are large, i.e. $L_d \sim 1$ (case of metals and materials with an opaque surface [14]); 2) light flow almost does not sustain losses when it passes through the material surface, i.e. $L_d \rightarrow 0$ (dielectrics) [15, 16];

The condition, at which the absorption constant is a function of the magnitude of a radiation flow q , i.e. $k = k(q)$, is often realized. We will consider just such a problem.

5. General solution of a one-dimensional problem of heat conductivity with allowance for the implicitly given absorption coefficient

In order to describe the processes on the surface of a solid substance, it is necessary to solve two differential equations with boundary conditions: namely, Eq. (5) with boundary condition (12) and also Eq. (7) with boundary condition (15). Equation (5) with boundary condition (12) evaluates elastic changes in the solid medium under an external irradiation action, and Eq. (7) with boundary condition (15) defines the thermal influence of radiation on the solid surface. Here, we will consider only problem (16) with boundary conditions (17) and (18).

Since we consider only the solid medium in the absence of fracture in this section, we omit the index "0" for simplicity.

The dependence of the energy flow q on the depth of penetration z into material is defined by the Lambert equation of the general form, where the coefficient of absorption $k(q)$ depends on the flow of radiation:

$$dq/dz = -qk(q),$$

where $k(q)$ is the absorption coefficient of a material. At this stage, we do not specify the coefficient of absorption and formulate problem (16)-(18) in the representation of a "quasispatial variable" $x = q/q_s$ [15], where q_s is the flow which has hit the surface of a solid substance. The variable x varies within the limits of $0 < x \leq 1$, inasmuch as the radiation flow q always decreases deep into a material ($q < q_s$).

In this representation, Eq. (19) becomes $x_z = -xk(x)$, where x_z stands for the derivative dx/dz . Then $\partial/\partial z = x_z \partial/\partial x$, and we can formulate Eq. (16) and boundary conditions (17), (18) in the new representation as

$$\rho C_v T_t = \lambda x_z \cdot (x_z T_x)_x - \mathcal{G}(\tau - t)(1 - L_d) q_s x_z, \quad (20)$$

$$T(0, x) = T_{in}, \quad T(t, 0) = T_{in},$$

$$T_x(t, 1) = L_d q_s \mathcal{G}(\tau - t) / (\lambda k(1)). \quad (21)$$

The ranges of definition of variables are as follows: $t \geq 0$, $0 < x \leq 1$. We solved system (20), (21) by applying the direct and inverse Laplace transformations with respect to time.

The gained solution describes the dynamics of the temperature of the surface which is warmed by a pulse of electromagnetic radiation. Namely:

$$\begin{aligned} T_s(t) = & T_{in} + \frac{2q_s}{(\pi\lambda\rho C_v)^{1/2}} \times \\ & \times \left\{ t^{1/2} \left[L_d + (1 - L_d) \cdot \int_0^1 \exp\left(\frac{\rho c(B(u))^2}{4\lambda t}\right) du \right] - \right. \\ & \left. - \frac{(\pi\rho C_v)^{1/2}}{2\lambda^{1/2}} (1 - L_d) \cdot \int_0^1 B(u) \operatorname{erfc}\left(\frac{(\rho c/\lambda)^{1/2}}{2t^{1/2}} B(u)\right) du \right\} - \\ & - \mathcal{G}(t - \tau) \frac{2q_s}{(\pi\lambda\rho C_v)^{1/2}} \times \\ & \times \left\{ (t - \tau)^{1/2} \left[L_d + (1 - L_d) \cdot \int_0^1 \exp\left(\frac{\rho c(B(u))^2}{4\lambda(t - \tau)}\right) du \right] - \right. \\ & \left. - \frac{(\pi\rho C_v)^{1/2}}{2\lambda^{1/2}} (1 - L_d) \cdot \int_0^1 B(u) \operatorname{erfc}\left(\frac{(\rho c/\lambda)^{1/2}}{2(t - \tau)^{1/2}} B(u)\right) du \right\}, \end{aligned} \quad (22)$$

where we denote $T_s(t) \equiv T(t, 1)$ and

$$B(x) = \int_x^1 \frac{dt}{tk(t)}. \quad (23)$$

In formula (22), the first three terms are responsible for the warming up of the surface during the action of a pulse, and the last two ones are included only then when the action of a pulse stops.

Relation (22) is the general solution for an arbitrary dependence of the absorption coefficient of a solid substance on the magnitude of a flow. The coefficient L_d takes the reflectivity into account; the surface value of the absorption coefficient is distinct from that in volume; the surface scattering is associated with a roughness of the surface and depends on the ratio between the incident radiation wavelength and the sizes of inhomogeneities of the surface and changes of the electron-phonon energetic structure of the surface. A specific feature of the obtained solution consists in that it allows determining the character of a nonlinearity of the radiation absorption in a material from the experimental measurement of the dynamics of the surface temperature and its comparison with Eq. (22). In this sense, it is possible to discuss the inverse problem of determination of $k(x)$ by the functional dependence $T_s(t)$ on the basis of the equation (22).

6. Approximation of the constant coefficient of absorption

Let's consider a case where the absorption coefficient is a constant: $k(x) = k_0$. Then relation (23) yields

$B(u) = -\ln(u)/k_0$. In this case, solution (22) after integration looks like

$$\begin{aligned} T_s^{k_0}(t) = & T_{in} + \frac{q_s}{\lambda k_0} \left(\frac{(at)^{1/2}}{\pi^{1/2}} + (1 - L_d) \cdot \right. \\ & \left. - \left[\exp(at/4) \operatorname{erfc}((at)^{1/2}/2) - 1 \right] \right) - \mathcal{G}(t - \tau) \times \\ & \times \frac{q_s}{\lambda k_0} \left(\frac{(a(t - \tau))^{1/2}}{\pi^{1/2}} + (1 - L_d) \times \right. \\ & \left. \times \left[\exp(a(t - \tau)/4) \operatorname{erfc}((a(t - \tau))^{1/2}/2) - 1 \right] \right), \end{aligned} \quad (24)$$

where $\alpha \equiv 4k_0^2\lambda(\rho C_v)$.

This dependence for the temperature dynamics in the case where the absorption coefficient is constant ($k_0 = \text{const} < \infty$) corresponds to the dependence $T_s(t)$ derived in work [17] for $L_d = 0$, i.e. when a surface is completely transparent for radiation.

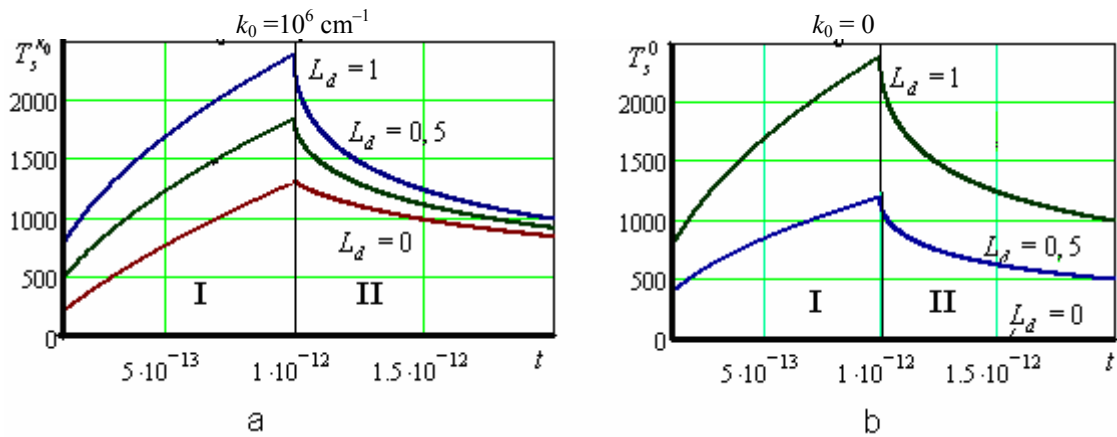


Fig. 1. Change of the surface temperature with time depending on the coefficient L_d of surface losses for aluminum during the action of a pulse (area I) and when the action of the pulse is completed (area II).

In the approximation $k_0 \rightarrow \infty$ (this is justified, for example, for metals at optical frequencies), the behavior of the temperature will be determined by a simpler equation

$$T_s^\infty(t) = T_{in} + \frac{2q_s L_d}{(\pi \lambda \rho C_V)^{1/2}} (t^{1/2} - \mathcal{G}(t - \tau)(t - \tau)^{1/2}). \quad (25)$$

For materials which do not absorb radiation (the volumetric coefficient of absorption $k_0 = 0$), the change in the surface temperature under irradiation is determined by the expression

$$T_s^0(t) = T_{in} + \frac{2q_s L_d}{(\pi \lambda \rho C_V)^{1/2}} (t^{1/2} - \mathcal{G}(t - \tau)(t - \tau)^{1/2}). \quad (26)$$

The dependence $T_s^0(t)$ differs from $T_s^\infty(t)$ only by the presence of a multiplier L_d and completely disappears in the absence of losses on the surface ($L_d = 0$), which is physically the exact result. The case where $L_d = 1$ is equivalent to the case of the infinite absorption coefficient (25).

Figure 1 shows the result of theoretical calculations of the dynamics of the temperature of a solid substance surface under the action of a laser pulse with the duration $\tau = 10^{-11}$ s and the intensity $q = 5 \cdot 10^9$ W/cm² for different values of the volume absorption coefficient k_0 and the coefficient of dissipative losses L_d . Thus, Fig. 1a gives the results of calculations according to relation (24) for a finite volume absorption coefficient k_0 , and Fig. 1b corresponds to formula (26) when the volumetric absorption constant is not considered. By comparing Fig. 1a and 1b, it becomes evident that, in the ideal case of a surface completely nontransparent for radiation ($L_d = 1$), the dynamics of the temperature does not depend on the volumetric absorption constant k_0 . If

$L_d < 1$, the value k_0 is a parameter which determines the surface heating. It is seen that the lowering of the temperature is running more slowly after the completion of the action of a pulse, than its growth during the irradiation.

Thus, the increase of the coefficient of dissipative superficial losses leads to a more essential local warming up of the surface of a solid substance. Hence, by varying the surface properties of a material and the properties of a coating which can be on the solid surface, we get possibility to additionally regulate its heating.

7. Conclusion

Thus, we have presented the general approach to the problem of the destructive or nondestructive treatment of a solid surface. The generalized boundary conditions are formulated, and it is shown that the problem can be divided into two independent problems. The first corresponds to the case without destruction of the surface. It defines the local changes of surface properties under the action of a laser pulse prior to the beginning of its destruction. Another problem deals with the destruction. It determines the dynamics of a spread of the gas phase during the destruction of a surface. We have considered the first problem. The attention has been paid to the energy equation which is transformed to the heat equation which considers the action of an exterior flow and defines changes of the surface temperature during the irradiation.

The generalized solution of the heat equation for an arbitrary dependence of the absorption coefficient of a solid substance on the magnitude of a flow is obtained. A specific feature of this solution consists in that it allows determining the character of a nonlinearity of the absorption in a material, by comparing the obtained solution with experimental data. This solution enables one to define, though at a phenomenological level, how the properties of the surface of a substance can influence a local site of the surface at the laser irradiation.

We have analyzed the dynamics of the substance surface temperature for three cases (two of which are the complete idealization): the infinite value of the coefficient of absorption of the radiation by a substance ($k_0 \rightarrow \infty$), a finite absorption coefficient, and a case where the coefficient of volumetric absorption is not taken into account ($k_0 = 0$). It is established that the rate of growth of the surface temperature depends on the absorption coefficient.

It is found that the influence of the surface properties of a substance is essential: with increase in the absorption coefficient and the coefficient of dissipative surface losses (under other identical conditions), the temperature of a surface will grow.

It is shown that the account of the absorption coefficient and the coefficient of surface losses changes essentially (sometimes by one hundred per cent) the peak value of the surface temperature, especially with increase in the radiation intensity, which should be taken into account in experiments with the use of powerful short pulses with $q \geq 10^{12}$ W/cm².

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