GENERAL QUESTIONS OF THERMODYNAMICS, STATISTICAL PHYSICS, AND QUANTUM MECHANICS

NONLINEAR DYNAMICS OF PRESSURE NEAR A SURFACE OF SUBSTANCE DURING LASER IMPULSE ACTIVITY

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We have studied the dynamics of a plasma plume under a destructive treatment. The main parameter determining the process is pressure. In the technologically relevant approximation when polytropic exponent is close to unity, the equation describing the dynamics divides into two ones which describe, respectively, the processes running during the destructive pulse action and after the termination of a pulse. The dependences of pressure on both the pulse duration and a parameter responsible for the radiation-gas interaction are analyzed.

1. Introduction

The problems of the interaction of powerful pulses of radiation with a surface are of great interest till now [1] [5]. In this case, the theoretical modeling of appropriate physical processes [1] is of great importance, because it allows one to clarify the nature of these processes. One of the important consequences of the action of a powerful pulse of radiation on a surface is the formation of a gas plume that arises due to a quick heating of the substance surface and, as a consequence, the destruction of this surface owing to phase transitions. In this article, we continue the development of a model of the interaction of pulses with a surface [6]. In particular, we study the specific features of both the surface destruction of a material and the space-temporal dynamics of a gas phase.

2. Influence of Radiation Absorption on the Dynamics of Pressure

During the action of radiation on a surface, there is the coexistence of the two, solid and gas, media due to local phase transitions. Using three boundary conditions, namely [6],

– the mass flux balance

$$\rho_s \left(\boldsymbol{v}_s \cdot \mathbf{n} \right) - \rho_s^{\text{sol}} \left(\boldsymbol{v}_s^{\text{sol}} \cdot \mathbf{n} \right) = 0, \tag{1}$$

— the momentum flow balance

$$P_{s}n_{i} + \frac{1}{c} \left(\mathbf{n} \cdot \mathbf{q}_{s} \right) + \rho_{s} \left(\mathbf{n} \cdot \boldsymbol{v}_{s} \right) \left(\boldsymbol{v}_{s}^{i} - \left(\boldsymbol{v}_{s}^{\text{sol}} \right)_{s}^{i} \right) + \left(P_{ij}^{\text{sol}} \right)_{s} n_{j} = 0$$

$$(2)$$

— and the energy flow balance near the interface

$$(\mathbf{n} \cdot \boldsymbol{v}_s) \left(\rho_s H_s + \rho_s \frac{v_s^2}{2} \right) + L_d \left(\mathbf{n} \cdot \mathbf{q}_s \right) - L\lambda_s (\mathbf{n} \cdot \operatorname{grad} T)_s + (\mathbf{n} \cdot \boldsymbol{v}_s) \rho_s \varphi_0 = 0,$$
(3)

has allowed us to formulate three equations which are characterized, in the main, by gas parameters and describe the dynamics of a crater formation, Eq. (1), the dynamics of a gas flame formation, Eq. (2), and the dynamics of the basic macroscopic quantities of the process, Eq. (3).

In Eqs. (1)–(3), U, ρ , and v are, respectively, the intrinsic energy of the continuous medium per unit mass, the density of this medium, and the convection

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velocity vector, P is the pressure acting on the system, $\left(P_{ij}^{\rm sol}\right)_s$ is the surface value of the stress tensor, H_s is the heat Gibbs function (enthalpy) describing a state of the macroscopic system in a thermodynamic equilibrium when entropy and pressure are the main independent variables, $U_s^{\rm sol}$ is the intrinsic energy of the condensed matter per unit mass; $\mathbf{Q} = \mathbf{q}_s + \mathbf{q}_s^{\rm T}$ is the general energy flow in the medium, where \mathbf{q}_s is the energy of a light flow and $\mathbf{q}_s^T \equiv -\lambda_s (\text{grad T})_s$ is the energy of a thermal flow, and L_d and L are, respectively, the loss factors of the light flow and the thermal flow under the transition from the gas to the solid.

We have examined the dynamics of a plasma plume under a destructive treatment. In this case, the fundamental parameter determining the dynamics of the process is pressure. In the general case, we have obtained the differential equation describing the pressure dynamics [8], namely

$$\frac{\partial \Pi}{\partial \theta} = \left(-1 + \Lambda e_q \vartheta_\tau\right) \Pi^{\beta+\eta} - \Pi^{\beta+1} + \frac{1}{N} e_q \vartheta_\tau \Pi^\eta, \qquad (4)$$

where $\beta \equiv \alpha/(2\kappa) \equiv (\kappa + 1)/(2\kappa)$, $\eta \equiv 1/\kappa$, Π is the dimensionless surface pressure, and Λ is a dimensionless parameter which is responsible for the gas-radiation interaction and significantly influences the pressure,

$$\Lambda = \frac{bL\gamma^3 q_{\rm in}}{2\varkappa\alpha\varphi_0} h(\omega). \tag{5}$$

Here, $b \equiv 2R_{\Gamma}m_a^2/(3\pi\sqrt{\pi}\gamma\mu_a d_a^2k_B)$, φ_0 is the specific heat of the condensate—gas phase transition, R_{Γ} is the gas constant; μ_a is the molecular weight of a gas; d_a is the effective diameter of a molecule; m_a is the mass of an atom of the evaporated matter, k_B is the Boltzmann constant, $\gamma \equiv \varkappa - 1$, \varkappa is the polytropic exponent, and the quantity $h(\omega)$ determines the constant part of the absorption factor which does not depend on pressure, but essentially depends on the frequency characteristics of the gas medium.

In Eq. (4), $\vartheta (\tau - t) \equiv \vartheta_{\tau}$ is the Heaviside's step function. This factor will limit the light-gas interaction time. The presence of partial derivatives is conditioned by the factor $1/N \equiv \left(\sqrt{1 + (\partial \Sigma/\partial x)^2 + (\partial \Sigma/\partial y)^2}\right)^{-1}$ depending on the space variables. The nonlinearity of the equation is characterized, besides the power function of pressure, by the unknown parameter e_q which can be

$$e_q = f(x, y) \exp\left(-\Lambda \Pi^{\eta + \beta} \Sigma\right).$$
(6)

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written in the dimensionless form as



Fig. 1. $\overline{\Pi}(\Lambda)$ dependence for the effective dimensionless pulse lengths $\theta_{\tau} = 10^5$ which corresponds to the real pulse length $\tau \sim 100 fs$ (left side) and $\theta_{\tau} = 10^{12}$ which corresponds to $\tau \sim 1\mu s = 10^{-6} s$ (right side)

Here, f(x, y) is the amplitude function; Π , θ , and Σ are, respectively, the dimensionless pressure, time, and a function which determines the crater surface form.

As one can see from Eq. (6), the e_q dependence on Λ , Π , and Σ is enough complicated. Moreover, the normal N, which enters into Eq. (4), also depends on Σ . All this makes the analysis of this equation too complicated. Therefore, we consider a particular case of the process which is described by Eq. (4) introducing some assumptions. First of all, we consider a situation, when the incident beam width is much more than the crater depth. This allows us to neglect the coordinate dependence of the crater form S at least at distances far from the crater edge and means that the term with 1/N will be absent in Eq. (4). In this case, due to the absence of a transverse pulse structure, the parameter e_q loses the dependence on the amplitude function f(x, y)(it is equal to unity) and can be determined in the case $\varkappa \to 1$ as $\bar{e}_q = \exp\left(-\Lambda \bar{\Pi}^2 \bar{\Sigma}\right)$, where \bar{e}_q , $\bar{\Pi}$, $\bar{\Sigma}$ are the average values of the corresponding functions. In other words, as $\varkappa \to 1$, Eq. (4) can be approximately written in the form [8]

$$\frac{d\Pi}{d\theta} = \left(-1 + \Lambda \bar{e}_q \vartheta_\tau\right) \Pi^2 - \Pi^2 + \bar{e}_q \vartheta_\tau \Pi.$$
(7)

Due to the properties of the Heaviside function, Eq. (7) breaks out into two separate equations, each of which is responsible for a part of the process depending on time:

1) $d\Pi_1/d\theta = ((-2 + \Lambda \bar{e}_q) \Pi_1 + \bar{e}_q) \Pi_1$ at $\theta \leq \theta_\tau \equiv \tau/t_o$ with the initial condition $\Pi_1(0) = \Pi_{\rm in}$.

2) $d\Pi_2/d\theta = -2\Pi_2^2$ at $\theta \ge \theta_\tau$.

The solution of the first equation for $\bar{e}_q = const$ in view of the initial condition is as follows:

$$\Pi_1\left(\theta\right) = \left(\left(\Pi_{\text{in}}^{-1} - 2\bar{e}_q^{-1} + \Lambda\right)\exp\left(-\bar{e}_q\theta\right) - \Lambda + 2\bar{e}_q^{-1}\right)^{-1}.$$
(8)

Further, we will analyze how the absorption of radiation by plasma influences the pressure due to their

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Fig. 2. Dependence $\overline{\Pi}(\theta_{\tau})$ at $\Lambda = 10^{-10}$

resonant interaction. Let us average Eq. (8) in the limits $0 \le \theta \le \theta_{\tau}$. As a result, we get

$$\overline{\Pi} = \frac{1}{2e^{\Lambda \overline{\Pi} \,^{3}\theta_{\tau}/2} - \Lambda} \times \left[1 + \left(\ln \left\{ e^{-\theta_{\tau} e^{-\Lambda \overline{\Pi} \,^{3}\theta_{\tau}/2}} + \Pi_{0} (2e^{\Lambda \overline{\Pi} \,^{3}\theta_{\tau}/2} - \Lambda) \times \right. \right. \\ \left. \times (1 - e^{-\theta_{\tau} e^{-\Lambda \overline{\Pi} \,^{3}\theta_{\tau}/2}}) \right\} \right) (e^{-\Lambda \overline{\Pi} \,^{3}\theta_{\tau}/2\theta_{\tau}})^{-1} \right],$$
(9)

where the explicit view of \bar{e}_q is taken into account, and it is assumed that $\overline{\Sigma} \simeq \theta_{\tau} \overline{\Pi}/2$. Inasmuch as the radiation absorption in plasma is characterized by the parameter Λ (the more the Λ , the greater the absorption), we will search the $\Pi(\Lambda)$ dependence by using Eq. (2.). As seen, this equation for $\overline{\Pi}$ is transcendental, so it can be analyzed only numerically.

As the area of the interaction of radiation with a plasma plume extends in the course of time, the dependence $\bar{\Pi}_1(\Lambda)$ (fig. 1) has correct behavior practically. The numerical investigations demonstrate that such a behavior $\overline{\Pi}(\Lambda)$ is not changed as θ_{τ} increases. Thus, the pressure $\bar{\Pi}_1$ approximately depends on the product $\Lambda \theta_{\tau}$. That is, the product $\Lambda \theta_{\tau}$ is not changed for any fixed value of $\bar{\Pi}_1$. The additional dependence on θ_{τ} is essential for small pulses lengths (Fig. 2). In dimensional units, this product takes the form $\frac{\alpha \varkappa^{3/2} L_d}{2\varphi_0^2 \gamma} h(\omega) q_{\rm in}^2 \tau$. Thus, under every specific conditions of the experiment, the pressure depends on the product $q_{\rm in}^3 \tau$, $\left(\bar{P} \sim \frac{\gamma L_d^2 \sqrt{\alpha \varkappa}}{4\varphi_0^{5/2}} h(\omega) q_{\rm in}^3 \tau\right)$.

A change of the pressure at the beginning of the destruction is shown in Fig. 2, where the dependence $\bar{\Pi}_1(\Lambda)$ is considered.

As seen from Fig. 2, there is the region of practically zero values of the average pressure (very close to zero, but not smaller than $\bar{\Pi}_{in}$).



Fig. 3. Dependence $\overline{\Pi}(\theta_{\tau})$ on the logarithmic scale for various possible (by estimations) values of Λ

It is essential that, with increase in $q_{\rm in}$, this region of a curve $\bar{\Pi}_1(\theta_{\tau})$ is narrowed, i.e. the substance starts to react to the external laser action at smaller destructive lengths θ_{τ} . The experimental facts [9] also confirm such restrictions on the radiation pulse duration. We note that the region of almost zero $\bar{\Pi}_1(\theta_{\tau})$ exists for all values of Λ .

Similar dependences $\overline{\Pi}(\theta_{\tau})$ for various Λ are shown in Fig. 3.

The relation between the parameter Λ and the absorption constant k of a gas medium [10] is k = $\frac{q_{\rm in} \alpha^{3/2} \varkappa^{1/2}}{2b \gamma^2 \varphi_0^{3/2}} \frac{L}{L_d^2} \Lambda \Pi^{\eta+\beta} \sim 10^{12} \Lambda \,{\rm cm}^{-1}.$ It is clear that $\overline{\Pi}(\theta_{\tau})$ probably traces the dependence $\Pi_{\max}(\theta)$. On the use of scale factors [10], it is possible to estimate the thermodynamic quantities during the destruction of a surface. For example, the pressure near the surface of a sapphire crystal during its destruction by pulses with the intensity $q = 10^{14}$ W/cm² can be expressed as $P = \frac{\gamma^2 L_d q_{\rm in}}{2\alpha^{1/2} \varkappa \sqrt{\varphi_0}} \Pi \approx 10$ TPa. Accordingly, the temperature of a plasma plume will be $T = \frac{m_a \gamma^2 \varphi_0}{k_B \alpha \varkappa} P^{\gamma/\varkappa} \approx 5 \cdot 10^5 K$, and the expansion velocity of the gas phase $v = \sqrt{\frac{\gamma^2 \varphi_0}{\alpha \varkappa} P^{\gamma/\varkappa}} = 1.1 \cdot 10^6 \text{ cm/s}$ $10^6 \mathrm{cm/s}$ with experimental in agreement results [11]. In all curves in Fig. 3, the pressure grows rapidly with time θ at the beginning and then starts to decrease. The greater is Λ , the faster the pressure decreases. This is caused by that the interaction region created by the corrosive plume rises, and the radiation pulse undergoes the more and more losses with time. The obtained function $\Pi_1(\theta)$ (8) describes the process of active ejection of the solid matter into the gas phase

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until the action of the pulse falling onto the surface

stops.

As seen in Fig. 3, the pressure acquires the maximum value at some time θ_1 ($\theta_1 \leq \theta_{\tau}$):

$$\Pi_{\max}(\theta) = \Pi_1(\theta_1) = ((\Pi_{in}^{-1} - 2/\bar{e}_q + \Lambda) \times \exp(\bar{e}_q \theta_1) - \Lambda + 2/\bar{e}_q)^{-1}.$$
(10)

Influence of Resonant Absorption of 3. Radiation on the Dynamics of a Plume

Here, we investigate the dependence of pressure on the radiation frequency ω . With this purpose, we examine the absorption coefficient k for a one-dimensional task in detail. As long as we speak about the resonance absorption of electromagnetic radiation, this coefficient is defined in the linear approximation [12] as

$$k_l = \frac{\omega}{c} \frac{\pi e^2}{2m_e m_a} \rho \sum_{m(\neq l)} \frac{f_{ml} \Gamma_{ml}}{\omega_{ml} (\omega_{ml} - \omega)^2}.$$
 (11)

The index l means that the coefficient k is responsible for the atom excitation from state l in one of the states m, over which the summation is fulfiled, ω is the electromagnetic radiation frequency; c is the velocity of light in vacuum; e is the electron charge, m_e is its mass; ω_{ml} is the atom radiation absorption proper frequency for its transition from state l into state m (it is resonance frequency); f_{ml} is the oscillator strength for the transition $l \to m$; and Γ_{lm} is the level width. For gases, we have

$$\Gamma_{ml} = \frac{4\pi d_a^2}{m_a} \rho \left(\frac{k_B T}{m_a}\right)^{1/2}.$$

It is common knowledge that the temperature can be determined from the equation of state of the ideal gas in terms of pressure and density. Then we get

$$\Gamma_{ml} = \frac{4\pi d_a^2}{m_a} \left(\rho P\right)^{1/2}.$$

If the radiation emission frequency ω is close to one of the resonance frequencies ω_{ml} (a quasiresonance state of the system), then only one dominant term can be conserved in the expression for the absorption coefficient k_l . In this case, atoms prior to the excitation are in the ground state l = 0. Then the absorption coefficient takes the form

$$k = \rho \left(\rho P\right)^{1/2} \frac{2\pi e^2 d_a^2}{2cm_e} \frac{\omega f_{m0}}{\omega_{m0} \left(\omega_{m0} - \omega\right)^2}.$$
 (12)

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Fig. 4. Qualitative dependence of the maximum pressure Π_{max} on frequency ω for arbitrary values W and θ_1

As seen, the frequency parameter $h_m(\omega)$ in the onedimensional case can be defined as

$$h_{m}(\omega) \equiv \frac{2\pi^{2}e^{2}d_{a}^{2}}{cm_{e}m_{a}^{2}} \frac{f_{m0}\omega}{\omega_{m0}(\omega_{m0}-\omega)^{2}}.$$
(13)

The mentioned parameter enters into the term with the multiplier Λ , which takes the interaction between the evaporated gas and radiation into account and is defined by Eq. (5).

In order to investigate the frequency dependence of the pressure Π_{max} , we consider expression (5), which demonstrates the dependence of Λ on the radiation frequency, and (13). This allows us to determine Π_{max} as a function of the difference of the radiation frequency and the proper frequency of the gas absorption:

$$\Pi_{\max}(\omega) = (\Pi_{\min}^{-1} \exp(-\theta_1 \exp(-G)) + (2\exp(G) - G)(1 - \exp(-\theta_1 \exp(-G))))^{-1}.$$
 (14)

Here, $G \equiv W \frac{\omega}{\omega_{m0} (\omega_{m0} - \omega)^2}$ and $W \equiv \frac{bL\gamma^3 q_{\rm in}}{\varkappa \alpha \omega_0} \frac{\pi^2 e^2 d_a^2 f_{m0}}{cm_e m_e^2}$, where φ_0 is the specific heat of

 $\varkappa \alpha \varphi_0 = c m_e m_a^2$ the condensate—gas phase transition.

In Eq. (14), the frequency dependence of the parameter \bar{e}_q is also taken into account. The dependence $\Pi_{\rm max}$ is shown in Fig. 4.

Thus, the qualitative character of the evaporation intensity dependence on the incident radiation frequency is represented by Eq. (14). In this case, as we can see from Fig. 4, the pressure decreases, when the frequency ω approaches ω_{m0} , and formally becomes equal to zero at $\omega \equiv \omega_{m0}$, which is in qualitative accordance with the earlier obtained results [7]. But the purely resonance case, $\omega \equiv \omega_{m0}$, needs a special investigation because, in this case, the dependence of the coefficient of absorption k on ρ and P acquires a somewhat different form than that in Eq. (12).

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4. Conclusion

We have reported the dynamics of the superficial pressure. It is shown that its magnitude is changed with increase in the length of a plasma plume at the expense of the interaction of radiation with a plume which is determined by the parameter Λ (Fig. 1).

Our analysis of the dependence of pressure on the pulse length shows that there exists, possibly, a conservation law for the product of the pulse intensity and its length (Fig. 2). It is also demonstrated (Fig. 3) that pressure reaches its maximum during the action of a pulse, but the time moment when this maximum is attained does not necessarily coincide with the termination time of a pulse.

The maximum pressure value Π_{max} dependence on frequency characteristics (14) is presented in Fig. 4. It is shown that it is essential over the range of resonant frequencies (pressure falls near to zero).

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НЕЛІНІЙНА ДИНАМІКА ТИСКУ БІЛЯ ПОВЕРХНІ МАТЕРІАЛУ ПІД ДІЄЮ ЛАЗЕРНОГО ІМПУЛЬСУ

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Резюме

Розглянуто динаміку плазмового факела при руйнівній обробці. Основним параметром, що визначає динаміку процесу, є тиск. У технологічно-актуальному наближенні, коли показник політропи близький до одиниці, рівняння, що описує цю динаміку, розпадається на два, одне з яких описує процес під час дії руйнівного імпульсу, а друге – після закінчення дії цього імпульсу. Проаналізовано залежності тиску від тривалості імпульсу й від параметра, що визначає взаємодію випромінювання з газом.