Numerical simulation of Thermomechanical Effects in Absorbing Liquids upon Excitation by Pulsed Laser Radiation

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Using the method of numerically solving the equations of motion of continuous media in the Lagrange form, simulations of the processes of excitation of pulsed acoustic beams during heating of absorbing liquids under an action of pulsed laser radiation has been carried out. The calculation of three-dimensional fields of temperature, pressure, density and velocity under the action of laser pulses with Gaussian spatial profile has been performed.

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1. Introduction

When a pulsed laser beam acts on an absorbing medium, it is locally heated, thermally expanded, and an acoustic (shock) wave is generated. The processes of laser-induced generation of acoustic signals can be effectively investigated based on the numerical solution of the equations of motion for continuous media in the Lagrange form [1]. For many practically important cases, the solution of a one-dimensional (planar, cylindrical or spherical) problem that is adequate to the geometry of energy release in the medium is sufficiently informative [2–4]. However, the development of a three-dimensional model that makes it possible to investigate

thermomechanical processes in absorbing medium when exposed to laser beams of arbitrary spatial structure and pulse duration, remains an urgent problem. In this work, based on the solution of three-dimensional equations of motion of continuous media in the Lagrange form, a method is developed for solving the problem of thermomechanical action of laser pulses on absorbing liquids. The results, in particular, can be used in the study of interaction of pulsed laser radiation with biological tissues.

2. Theoretical model

The system of equations of motion of a continuous medium consists of the equation of continuity, the equations of motion, the equation of energy balance and the equation of state. In the Lagrangian formulation for three-dimensional

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motion, these equations have the form [5]:

• a continuity equation:

$$V = V_0 \left[\frac{\partial x_{\rm e}}{\partial x_{\rm l}} \left(\frac{\partial y_{\rm e}}{\partial y_{\rm l}} \frac{\partial z_{\rm e}}{\partial z_{\rm l}} - \frac{\partial y_{\rm e}}{\partial z_{\rm l}} \frac{\partial z_{\rm e}}{\partial y_{\rm l}} \right) - \frac{\partial y_{\rm e}}{\partial x_{\rm l}} \left(\frac{\partial x_{\rm e}}{\partial y_{\rm l}} \frac{\partial z_{\rm e}}{\partial z_{\rm l}} - \frac{\partial x_{\rm e}}{\partial z_{\rm l}} \frac{\partial z_{\rm e}}{\partial y_{\rm l}} \right) + \frac{\partial z_{\rm e}}{\partial x_{\rm l}} \left(\frac{\partial x_{\rm e}}{\partial y_{\rm l}} \frac{\partial y_{\rm e}}{\partial z_{\rm l}} - \frac{\partial x_{\rm e}}{\partial z_{\rm l}} \frac{\partial y_{\rm e}}{\partial y_{\rm l}} \right) \right]; \quad (1)$$

• equations of motion:

$$\frac{\partial^2 x_{\rm e}}{\partial t^2} \frac{\partial x_{\rm e}}{\partial x_1} + \frac{\partial^2 y_{\rm e}}{\partial t^2} \frac{\partial y_{\rm e}}{\partial x_1} + \frac{\partial^2 z_{\rm e}}{\partial t^2} \frac{\partial z_{\rm e}}{\partial x_1} = -\frac{1}{\rho} \frac{\partial P}{\partial x_1},\tag{2}$$

$$\frac{\partial^2 x_{\rm e}}{\partial t^2} \frac{\partial x_{\rm e}}{\partial y_{\rm l}} + \frac{\partial^2 y_{\rm e}}{\partial t^2} \frac{\partial y_{\rm e}}{\partial y_{\rm l}} + \frac{\partial^2 z_{\rm e}}{\partial t^2} \frac{\partial z_{\rm e}}{\partial y_{\rm l}} = -\frac{1}{\rho} \frac{\partial P}{\partial y_{\rm l}},\tag{3}$$

$$\frac{\partial^2 x_{\rm e}}{\partial t^2} \frac{\partial x_{\rm e}}{\partial z_{\rm l}} + \frac{\partial^2 y_{\rm e}}{\partial t^2} \frac{\partial y_{\rm e}}{\partial z_{\rm l}} + \frac{\partial^2 z_{\rm e}}{\partial t^2} \frac{\partial z_{\rm e}}{\partial z_{\rm l}} = -\frac{1}{\rho} \frac{\partial P}{\partial z_{\rm l}}; \tag{4}$$

• equations of the changing of Euler coordinates:

$$u_{x_{\rm e}} = \frac{\partial x_{\rm e}}{\partial t}, u_{y_{\rm e}} = \frac{\partial y_{\rm e}}{\partial t}, u_{z_{\rm e}} = \frac{\partial z_{\rm e}}{\partial t};$$
 (5)

• an equation of state:

$$P = P(V, E). (6)$$

Here, x_e, y_e, z_e are the Euler coordinates; P is the pressure; $V_0 = 1/\rho_0$, $V = 1/\rho$ are the initial and current specific volumes; ρ_0 , ρ are the corresponding densities; E is the specific internal energy.

As the equation of state of an absorbing liquid, the Mie–Grüneisen equation in its binomial (cold, and hot parts) form has been used [6]:

$$P = \rho_0 u_0^2 \left(1 - \frac{V}{V_0} \right) + \Gamma \frac{C (T - T_0)}{V}, \quad (7)$$

where Γ is the Grüneisen coefficient of the medium, u_0 is the sound speed in the medium.

To describe the heating of the medium upon absorption of laser radiation energy, the following heat conduction equation has been used:

$$\rho C \frac{\partial T}{\partial t} = k_T \left(\frac{\partial^2 T}{\partial x_l^2} + \frac{\partial^2 T}{\partial y_l^2} + \frac{\partial^2 T}{\partial z_l^2} \right) + Q_S. \quad (8)$$

Here, ρ is the density, C is the heat capacity of the medium, T is the temperature. The value of Q_S in equation (8) is determined by the energy release source: $Q_S = I\left(x_1, y_1, z_1, t\right) k_{abs}$, where k_{abs} is the absorption coefficient of the medium; $I\left(t, x_1, y_1, z_1\right) = I_0 f_t\left(t\right) f_{xyz}\left(x_1, y_1, z_1\right)$ is the intensity of the light beam at the moment t at a point in space with a coordinate (x_1, y_1, z_1) , the function $f_{xyz}\left(x_1, y_1, z_1\right)$ is determined by the law of absorption (below $f_{xyz}\left(x_1, y_1, z_1\right) = f_{yz}\left(x_l, y_l\right) \exp\left[-k_{abs}x_l\right]$). The time profile of laser pulse is described by a power-exponential function $f_t\left(t\right) = \frac{t}{\tau_p} e^{-\frac{t}{\tau_p}}$, where τ_p is the duration of the laser pulse.

Numerical modeling of the system of equations of motion in the Lagrange form was carried out using the method of finite-difference approximation described in [7] and adapted to the multidimensional case, taking into account

the introduction of pseudoviscosity, which made it possible to stabilize the numerical solution in the region of existence of pressure surges; heat conduction equation were solved according to the three-layer explicit scheme presented in [8]. When setting the boundary conditions, it was assumed that the boundary $x_1 = 0$ is a rigid boundary. When implementing the numerical method, the calculation area was divided into $200 \times 200 \times$ 200 cells. The time step was determined by the Courant criterion $\Delta t = k\Delta x_1/u_0$, where u_0 is the sound speed in the material, $k = 0.1 \div 0.01$.

3. Numerical results and discussion

The obtained system of equations allows one to describe the process of excitation of pulsed acoustic beams at arbitrary scales of absorbing structures. However, for efficient excitation of acoustic pulses, the duration of laser heating of the medium should be substantially shorter than the acoustic relaxation time of the heated volume. With a typical absorption coefficient of water in the neat IR region $k_{abs} = 10 \text{ cm}^{-1}$ and a speed of sound $u_0=1.5\cdot 10^5$ cm/s, the acoustic relaxation time is $t_a=\frac{1}{k_{abs}u_0}\approx 10^{-6}$ s. Thus, the pulse duration of laser sources effective for excitation of acoustic signals in such media can be estimated as a value on the order of tens to hundreds of nanoseconds.

Let us consider the processes of heating and excitation of acoustic pulses in an absorbing liquid (colored water, $k_{abs} = 10 \text{ cm}^{-1}$) placed in a cell (the boundary condition is a rigid boundary) under the action of pulsed laser radiation with parameters characteristic of the Q-switching mode. We assume that the intensity at the maximum of the Gaussian beam is $I_0 =$ $3.2 \cdot 10^7$ W/cm², and the duration of the laser pulse is $\tau_{\rm p} = 50$ ns. The radius of the Gaussian beam varied from $r_0 = 0.01$ cm to $r_0 = 0.2$ cm. Thus, the pulse energy varied from E = 2 mJ to E = 200 mJ.

The results of numerical simulation of this

problem are presented in Figures 1-3 in the form of pressure fields (in bars) calculated at successive times in the plane containing the light beam propagation coordinate and one of the transverse coordinates. Figure 1 shows the results of calculating the evolution of the pressure field in the case of a sharp focusing of the laser beam $(r_0 = 0.01 \text{ cm})$, while $r_0 k_{abs} = 0.1 < 1$, and one can speak of its large penetration depth into the absorbing medium. As can be seen, after the end of the action of the laser pulse (t =100 ns), an area of increased pressure is formed in the region of energy release. The subsequent relaxation of this perturbation (t > 200 ns)leads to the formation of a bipolar (compressionrarefaction) acoustic pulse, mainly in the cross section relative to the axis of propagation of the laser pulse. There is practically no generation of an acoustic pulse along the axis of propagation of the laser beam, and it can be said that the structure of the acoustic pulse is characterized by quasi-cylindrical symmetry. Note that under the conditions under consideration, the amplitude of the pressure wave is directly proportional to the intensity of the acting laser radiation over a wide range, and the speed of the propagating acoustic pulse is equal to the speed of sound in the medium. However, the general statement of the problem admits a solution up to pressure wave amplitudes corresponding to the formation of a shock wave in the medium.

Figure 2 demonstrates the spatiotemporal evolution of the pressure field in a medium under the action of a Gaussian laser beam with a radius $r_0 = 0.1$ cm. Other parameters (laser pulse duration, peak intensity, medium absorption coefficient) are the same as for the previous calculation. In this case, the product of the radius of the Gaussian beam and the absorption coefficient is equal to unity $(r_0k_{abs} =$ 1), which determines the quasi-spherical shape of the generated pressure wave.

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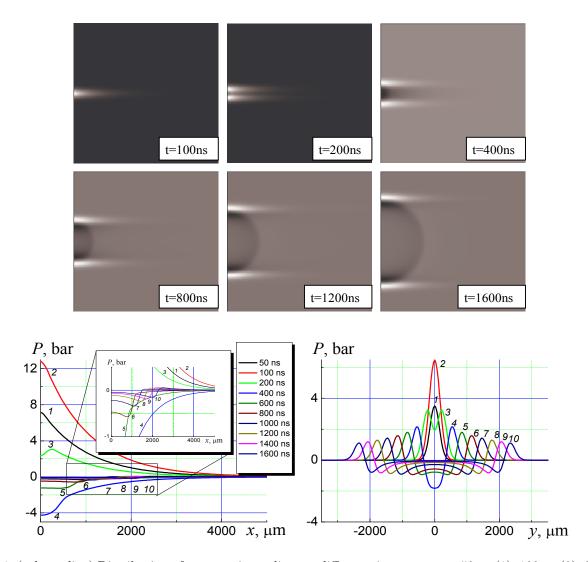


FIG. 1. (color online) Distribution of pressure in medium at different time moments: 50 ns (1), 100 ns (2), 200 ns (3), 400 ns (4), 600 ns (5), 800 ns (6), 1000 ns (7), 1200 ns (8), 1400 ns (9), 1600 ns (10). Laser beam radius $r_0 = 0.01$ cm.

(laser pulse duration, peak intensity, medium absorption coefficient) are the same as for the previous calculation. In this case, the product of the radius of the Gaussian beam and the absorption coefficient is equal to unity $(r_0k_{abs} = 1)$, which determines the quasi-spherical shape of the generated pressure wave. Note that, for the selected parameters of laser radiation, the amplitude of the pressure wave in the negative phase can already reach values sufficient for the formation of a cavitation bubble. Therefore, for a correct description of this phenomenon, it is

necessary to modernize the model. In this paper, we do not consider these issues.

A further increase inthe radius of beam, while the Gaussian laser keeping other parameters unchanged, leads to the implementation of condition $r_0 k_{abs} > 1$, which in turn allows us to consider the case of excitation of a quasi-planar acoustic beam. This situation is considered in Figure 3, which shows the spatiotemporal distributions of pressure in the medium for the radius of the Gaussian laser beam $r_0 = 0.2$ cm. As can be seen, in this case, after

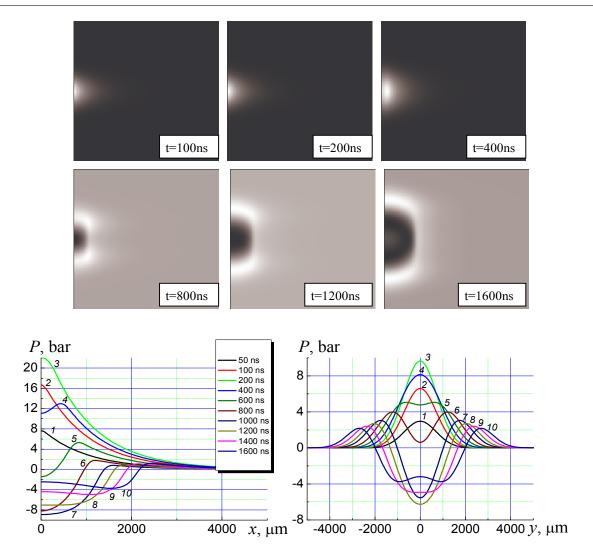


FIG. 2: (color online) The same as Fig. 1 but laser beam radius $r_0 = 0.1$ cm.

the transient process in the direction coinciding with the direction of laser beam propagation, a quasi-plane pressure wave is formed, which is characterized by the presence of compression and rarefaction phases.

We note that a significant difference between the results obtained in this work and the results obtained in one-dimensional models of the generation of plane-wave acoustic pulses with energy release near a rigid boundary is the prediction of the generation of bipolar (compression-rarefaction) pressure waves even for the case of very wide laser beams, precisely due to taking into account the finite width of the beams.

Conclusion

In conclusion, we note that the numerical experiments performed have shown the operability of the considered method for calculating thermomechanical processes absorbing media under an action of pulsed laser radiation in a wide range of pulse durations and for an arbitrary transverse beam profile. The results can be used in the problems of the impact of pulsed and repetitively pulsed laser radiation on biological tissues, in particular, for the development of physical principles of cavitation ("cold") laser surgery [9], which can be

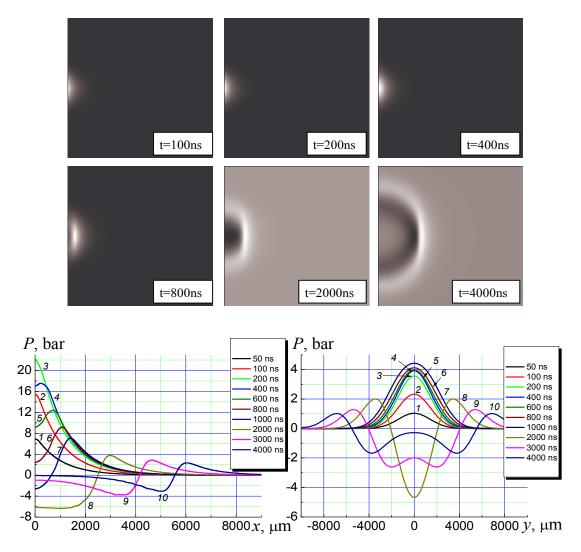


FIG. 3. (color online) Distribution of pressure in medium at different time moments: 50 ns (1), 100 ns (2), 200 ns (3), 400 ns (4), 600 ns (5), 800 ns (6), 1000 ns (7), 2000 ns (8), 3000 ns (9), 4000 ns (10). Laser beam radius $r_0 = 0.2$ cm.

used in ophthalmology as well [10].

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