# Numerical simulation of thermomechanical action of ultrashort laser pulses on metals

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**Abstract**

Physical, mathematical and numerical models of laser-induced excitation of acoustic pulses in metals have been developed to study the regularities of propagation of acoustic signals excited by ultrashort laser pulses of various spatial structures. The space-time structure of temperature fields and pressure waves excited in metals is simulated numerically, depending on the duration of laser pulses and the thermophysical characteristics of materials.

**Keywords**: ultrashort laser pulses, metals, numerical simulations.

## Introduction

The invention of lasers as new sources of electromagnetic radiation opened up wide opportunities for studying the processes of interaction of intense radiation with matter. Despite the past 60 years, this area of physics is still developing at extremely rapid steps. The phenomena of interaction of intense radiation with matter include many different effects, often completely different in nature: this is the generation of harmonics in nonlinear crystals, laser melting or destruction of materials, action on biological tissues, and many others [1]. The physics of the interaction of intense laser radiation with metals is especially rich [2]. Depending on the duration and intensity of laser radiation, the characteristic processes are heating, melting and evaporation of the target material, thermal and photoelectron emission, and the formation of high-temperature plasma. Accordingly, it is possible to implement various technological modes of action of laser radiation (cutting, welding, punching holes, etc.).

For the theoretical description of these phenomena, in accordance with the capabilities of modern computer technology, models of various levels of complexity are being developed, including the solution of nonlinear thermal problems, problems of describing phase transitions (melting, evaporation of a material), hydrodynamic problems associated with both thermal convection of a melt and the dynamics of plasma cloud expansion.

The interaction of ultrashort laser pulses (pico- and femtosecond duration) with metals is currently an area of research with numerous potential or already realized applications. As a rule, in times of the order of tens - hundreds of femtoseconds, the electron gas is heated, followed by relaxation of the excitation energy into the ionic subsystem. Further dynamics of the ionic lattice is determined by the initial localization and further propagation of acoustic deformations, which have a characteristic scale (units - tens of nanometers) associated with the depth of radiation penetration into the metal. The generation of such spatially localized perturbations is promising for such applications as, for example, non-destructive testing of the parameters of materials in the nano- and micro-range.

The main goal of this work is the development of theoretical and numerical models that would make it possible to analyze temperature fields, pressure fields, density and velocity of material movement when exposed to ultrashort laser pulses of various spatial structures (Gaussian, vortex, and Bessel beams). Further development of this model, associated with the inclusion in the description of the phenomenon of metal melting, will make it possible to get as close as possible to the description of the processes of formation of regular and irregular micro- and nanostructures on the metal surface.

**Theoretical model**

A theoretical consideration of the interaction of ultrashort laser pulses with metals requires the development of models that take into account the essentially nonequilibrium nature of the process of laser heating of metals. Heating of a metal layer under the action of ultrashort laser pulses can be described within the framework of a two-temperature model for electron gas and ionic lattice [2]:

$$\rho_e C_e \frac{\partial T_e}{\partial t} = k_T^e \left( \frac{\partial^2 T_e}{\partial x^2} + \frac{\partial^2 T_e}{\partial y^2} + \frac{\partial^2 T_e}{\partial z^2} \right) + Q_S - \gamma \left( T_e - T_i \right), \tag{1}$$

$$\rho_i C_i \frac{\partial T_i}{\partial t} = \gamma \left( T_e - T_i \right). \tag{2}$$

Here the values $\rho$ (density), $C$ (heat capacity), $T$ (temperature), $k_T$ (thermal conductivity) with the index "*e*" refer to the electronic subsystem, with the index "*i*" - to the ionic one. The parameter $\gamma$ determines the rate of energy relaxation from the electron gas to the ions of the crystal lattice. The value $Q_S$ is determined by the source of energy release: $Q_S = \kappa I_0 \dfrac{t}{\tau_p} e^{-t/\tau_p}$, where $I_0$ is the intensity of the light beam, $\kappa$ is the absorption coefficient of the medium, and $\tau_p$ is the duration of the laser pulse.

Under the action of pulsed laser radiation on the absorbing medium, its local heating, expansion and generation of an acoustic pulse occurs. These processes can be effectively modeled by numerically solving the equations of motion of the medium in the form of Lagrange.

The continuity equation has the form:

$$V = V_0 \left[ \begin{array}{l} \dfrac{\partial x_e}{\partial x_l}\left( \dfrac{\partial y_e}{\partial y_l}\dfrac{\partial z_e}{\partial z_l} - \dfrac{\partial y_e}{\partial z_l}\dfrac{\partial z_e}{\partial y_l} \right) - \\ - \dfrac{\partial y_e}{\partial x_l}\left( \dfrac{\partial x_e}{\partial y_l}\dfrac{\partial z_e}{\partial z_l} - \dfrac{\partial x_e}{\partial z_l}\dfrac{\partial z_e}{\partial y_l} \right) + \dfrac{\partial z_e}{\partial x_l}\left( \dfrac{\partial x_e}{\partial y_l}\dfrac{\partial y_e}{\partial z_l} - \dfrac{\partial x_e}{\partial z_l}\dfrac{\partial y_e}{\partial y_l} \right) \end{array} \right], \tag{3}$$

where, $V_0 = 1/\rho_0$, $V = 1/\rho$ - initial and current specific volumes; $(x_l, y_l, z_l)$ - Lagrangian coordinates; $(x_e, y_e, z_e)$ - Euler coordinates.

The equations of motion, assuming the absence of external forces, are written in the form:

$$\frac{\partial u_{x_e}}{\partial t} = -V_0 \left[ \begin{array}{l} \dfrac{\partial P}{\partial x_l}\left( \dfrac{\partial y_e}{\partial y_l}\dfrac{\partial z_e}{\partial z_l} - \dfrac{\partial y_e}{\partial z_l}\dfrac{\partial z_e}{\partial y_l} \right) - \\ - \dfrac{\partial y_e}{\partial x_l}\left( \dfrac{\partial P}{\partial y_l}\dfrac{\partial z_e}{\partial z_l} - \dfrac{\partial P}{\partial z_l}\dfrac{\partial z_e}{\partial y_l} \right) + \dfrac{\partial z_e}{\partial x_l}\left( \dfrac{\partial P}{\partial y_l}\dfrac{\partial y_e}{\partial z_l} - \dfrac{\partial P}{\partial z_l}\dfrac{\partial y_e}{\partial y_l} \right) \end{array} \right], \tag{4}$$

$$\frac{\partial u_{y_e}}{\partial t} = -V_0 \left[ \begin{array}{l} \dfrac{\partial x_e}{\partial x_l}\left( \dfrac{\partial P}{\partial y_l}\dfrac{\partial z_e}{\partial z_l} - \dfrac{\partial P}{\partial z_l}\dfrac{\partial z_e}{\partial y_l} \right) - \dfrac{\partial P}{\partial x_l}\left( \dfrac{\partial x_e}{\partial y_l}\dfrac{\partial z_e}{\partial z_l} - \dfrac{\partial x_e}{\partial z_l}\dfrac{\partial z_e}{\partial y_l} \right) + \\ + \dfrac{\partial z_e}{\partial x_l}\left( \dfrac{\partial x_e}{\partial y_l}\dfrac{\partial P}{\partial z_l} - \dfrac{\partial x_e}{\partial z_l}\dfrac{\partial P}{\partial y_l} \right) \end{array} \right], \tag{5}$$

$$\frac{\partial u_{z_e}}{\partial t}=-V_0\left[\begin{array}{l}\frac{\partial x_e}{\partial x_1}\left(\frac{\partial y_e}{\partial y_1}\frac{\partial P}{\partial z_1}-\frac{\partial y_e}{\partial z_1}\frac{\partial P}{\partial y_1}\right)-\frac{\partial y_e}{\partial x_1}\left(\frac{\partial x_e}{\partial y_1}\frac{\partial P}{\partial z_1}-\frac{\partial x_e}{\partial z_1}\frac{\partial P}{\partial y_1}\right)+\\ +\frac{\partial P}{\partial x_1}\left(\frac{\partial x_e}{\partial y_1}\frac{\partial y_e}{\partial z_1}-\frac{\partial x_e}{\partial z_1}\frac{\partial y_e}{\partial y_1}\right)\end{array}\right]. \tag{6}$$

The equations for changing the Euler coordinates are written as follows:

$$u_{x_e}=\frac{\partial x_e}{\partial t},\ u_{y_e}=\frac{\partial y_e}{\partial t},\ u_{z_e}=\frac{\partial z_e}{\partial t}. \tag{7}$$

To approximate the equation of state of the metal layer, we use Mie-Grüneisen equation, which takes the form [3]:

$$P=\rho_{i0}u_0^2\left(1-\frac{V_i}{V_{i0}}\right)+\Gamma_i\frac{C_i\left(T_i-T_0\right)}{V_i}+\Gamma_e\frac{C_e\left(T_e-T_0\right)}{V_e}, \tag{8}$$

where, $V_{i0}$, $V_{i,e}$ are the initial and current specific volumes, $V_{i0}=1/\rho_{i0}$, $V_{i,e}=1/\rho_{i,e}$, where, $\rho_{i0}$, $\rho_{i,e}$ are the corresponding densities, $\Gamma_{i,e}$ are the Grüneisen coefficients, $u_0$ is the speed of sound in the metal layer.

**Results and discussion**

Numerical modeling was carried out under the assumption of the action of an ultrashort laser pulse (intensity of the order of $I_0$=$10^8$W/cm$^2$, duration of the order of $\tau_p$=$10^{-13}$s) on the gold layer (absorption coefficient $\kappa$=$5\cdot10^5$cm$^{-1}$). The calculations were performed for typical thermophysical parameters of Au. When solving the thermal problem, all parameters of the material were considered constant, without taking into account their temperature dependence. As follows from the test calculation for the one-dimensional geometry of the problem presented on Figure 1, with the used material parameters, the establishment of temperature equilibrium of two subsystems (electronic and ionic) occurs in times of the order of 10ps.

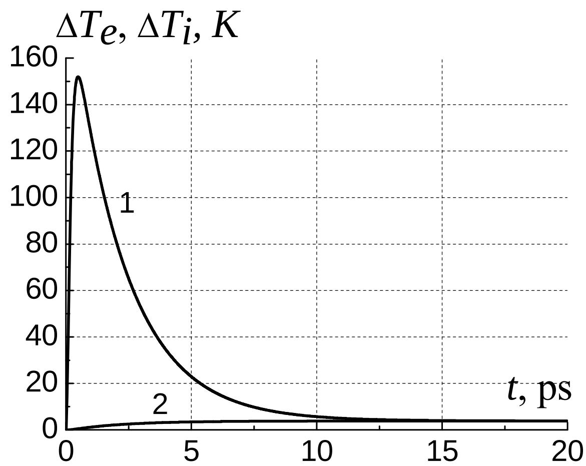
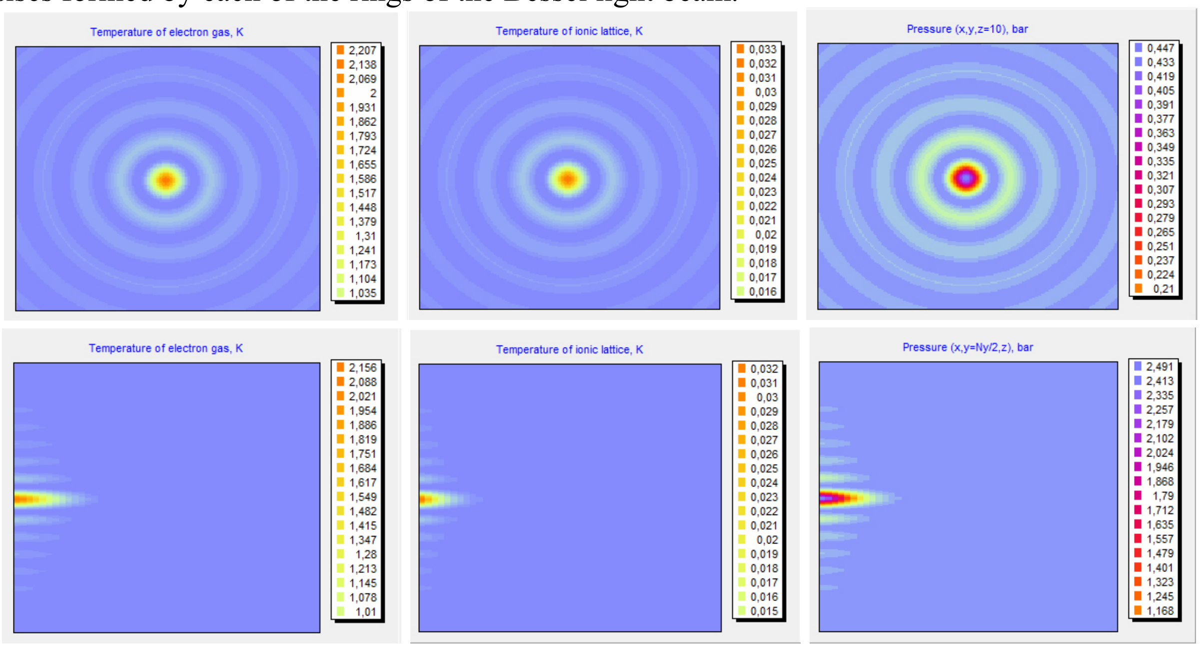



Figure 1. Time dependences of changes in the temperature of the electronic (1) and ionic (2) subsystems on the surface of the metal (Au) layer

Numerical experiments on calculating the structure of an acoustic pulse generated in a metal layer were carried out for various transverse structures of laser beams (Gaussian, vortex, Bessel).

Below, we present the results of a numerical solution of the system of equations of motion under the assumption that an ultrashort laser pulse acts on the metal layer; the intensity distribution in a cylindrically symmetric transverse profile is modeled by the square of the Bessel function of order $m$: $I(r) \sim J_m^2(r/r_0)$. It is assumed in the calculations that $m=0$, $r_0 = 100 \mu m$. The spatial distributions of temperature and pressure after the end of the laser pulse are shown in Figure 2. Further evolution of the acoustic wave field demonstrates the propagation of two components in the directions along the laser beam propagation axis and in the cross section. Moreover, a cylindrical pressure wave propagates in the cross section, consisting of a sequence of compression - rarefaction pulses formed by each of the rings of the Bessel light beam.




(a)

(b)

Figure 2. Distribution of the temperature of the electron gas, the temperature of the ionic lattice, the pressure in the near-surface layer of the metal in the section perpendicular to the direction of propagation of the zero-order Bessel light beam (a), and in the section containing the axis of propagation of the zero-order Bessel light beam (b), at the time moment t=1000fs from the beginning of the action of the laser pulse

**Conclusion**

The developed model makes it possible to evaluate the results of the thermomechanical action of ultrashort laser pulses on metal layers. It is shown that the structure of the excited acoustic signals is a train of compression - rarefaction waves, the structure of which is determined by the spatial structure of the laser beam.

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**References:**

[1] J. Ready, Effects of high-power laser radiation. Academic Press (1971) 468p.
[2] S.I. Anisimov, Ya.A. Imas, G.S. Romanov, and Yu.V. Khodyko, The Effect of High Power Radiation onto Metals. Moscow: Nauka, (1970) 272p.
[3] O.G. Romanov, G.I. Zheltov, and G.S. Romanov, Bull. of the RAS: Physics, V.75 (2011) P.1589-1591.