Research and modeling of laser ablation by ultra-short laser pulses for metal targets

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Abstract. In this article an improved mathematical model for a laser metal ablation by ultra-short duration laser pulses is proposed. The model is based on two-temperature hydrodynamic model for electrons and ions and wide-range equation of state for metals. The results of the computer simulation for aluminum and copper are compared with experimental data at a different laser fluence and duration of pulses for ablation depth. A good agreement with them and the experimental data of ablation depth is received.

1. Introduction

Nowadays, laser material processing, especially by ultra short duration pulses (pico or femtosecond), is an effective way for a micromachining and nano-machining [1, 2], structural modification of the material surface [3] and for the material removal of different solid materials (which is called ablation) [4] because of the small affected zone and enough well reproducibility. The absorption of the laser radiation with ultra short duration pulses goes mainly at the material interface and the deposition of the laser energy and removing the upper layer of the material are also goes significantly faster than in the main part of it. So, the laser ablation proceeds with small secondary damage to the surrounding material, in opposite to nanosecond laser ablation [5].

Initially, the laser radiation energy in metals is absorbed by the free or weakly bound electrons. After that in some femtoseconds gas of electrons is thermalized by electron–electron collisions. Then electron–lattice relaxation takes place (in a several picoseconds) and the emission of particles, which have gained enough energy, is occurring. For the metals such physical processes and their approximate time scales are shown in Figure 1.

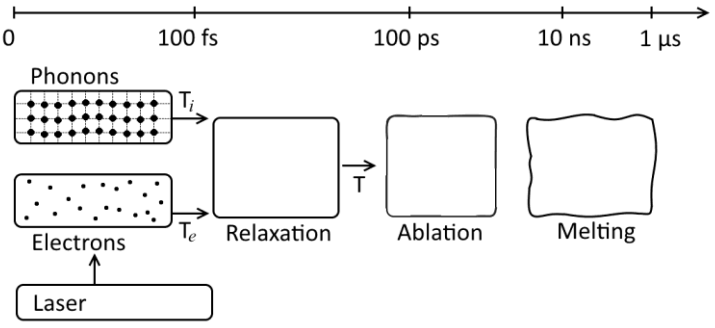

Figure 1. Processes and approximate time scales for metal ablation by about 100 fs duration laser pulse.

But the prediction of the changes in the material after the laser ablation is happened (even the depth of the ablation crater after the material removal) is hard to make properly, because they are depending on many factors – laser radiation characteristics, type of the material and surrounding medium [6, 7]. So, this task is relevant for a mathematical modeling in different cases [8-11].

For the computer simulation of laser ablation, two main approaches are used now - molecular dynamic models and continuous thermodynamic models. In the first approach trajectories of particles are found by numerical solution of the system of the motion equations for all of them with using the chosen interatomic potential of interaction that is responsible to thermodynamic properties and the equilibrium structure of the material [12]. An important advantage here is that no (of few) further assumptions on the processes are required for calculations, but simulation requires a lot of computational resources, which significantly limits the size of the study area or time frame of the processes under research [13]. In the second approach a mathematical model in two temperature form is often used for the simulation of ultra-short laser processing [14]. In this model the energy transfer in the metal is described by two coupled generalized equations of heat conduction (with different the electrons and the lattice temperatures). The material removal processes in this model are often described by a system of hydrodynamic equations. However, when interaction between material and laser radiation is studied, an appropriate calculation for the thermodynamic material properties is required over a wide region of states including normal condition or even plasma state at high pressures and temperatures [15, 16]. In addition, hybrid models are also being used for simulation, but the coordinated and physically correct work of the sub-components responsible for thermodynamic and molecular-dynamic calculations in them is a rather complicated task [17].

Therefore, there is still a need to develop a mathematical model for the rather quickly and enough accurately computer simulation of laser ablation. In our article we propose an improved mathematical model [18] in two temperature form with using the wide-range two-temperature equation of state for receiving better accuracy.

2. Mathematical model

The mathematical model for laser ablation is proposed in the two-temperature form based on conservation laws - for the mass, for the momentum and the energy of electron and ion subparts:

$$\frac{\partial}{\partial t}\left(\frac{1}{\rho}\right)+\frac{\partial v}{\partial m}=0 \tag{1}$$

$$\frac{\partial v}{\partial t}+\frac{\partial P}{\partial m}=0 \tag{2}$$

$$\frac{\partial \varepsilon_e}{\partial t}+P_e\frac{\partial v}{\partial m}=-\frac{a_{ei}}{\rho}(T_e-T_i)+\frac{\partial}{\partial m}\left(k\rho\frac{\partial T_e}{\partial m}\right)+I \tag{3}$$

$$\frac{\partial \varepsilon_i}{\partial t}+P_i\frac{\partial v}{\partial m}=\frac{a_{ei}}{\rho}(T_e-T_i) \tag{4}$$

here m - the mass coordinate, v - the velocity, t is the time, ρ - the density, T_e and T_i, ε_e and ε_i, P_e and P_i - the temperatures, internal energies, pressures of electrons and ions, $P=P_e+P_i$ and $\varepsilon=\varepsilon_e+\varepsilon_i$ - the sums of the pressure and the internal energy, a_{ei} - electron-ion relaxation coefficient, I - absorbed laser radiation energy, given by formula based on Beer–Lambert law:

$$I=\frac{B}{\tau_L\delta\sqrt{\pi}\rho}\exp\left(\frac{x(m_0,t)-x(m,t)}{\delta}\right)\exp\left(-\frac{t^2}{\tau_L^2}\right) \tag{5}$$

where B is the laser radiation energy, τ_L - the duration of the laser pulse, δ - the metal skin depth, $x(m,t)$ - particle trajectory with coordinate m, m_0 - metal surface coordinate.

To solve the system of hydrodynamic equations in this mathematical model we supplement it with equation of state for metals in wide-range two-temperature form, where to describe the thermodynamic properties of a metal (pressure, internal energy and temperature) the free energy is used. For a numeric cell it is described as sum of the electronic and ionic components, and the part responsible for the interaction between them:

$$F=F_e+F_i+F_{ei} \tag{6}$$

Cell volume V and temperatures T_e, T_i are used as main thermodynamic parameters. The electron pressure is described as the ideal Fermi electron gas pressure with temperature T_e and density y/V, where y is received by solving the slightly modified equation of ionization:

$$\mu_F\left(\frac{y}{V},T_e\right)+I(y)-b\left(\frac{Z}{V}\right)^{\beta}(1+\mu T_e V^{\sigma})^{-1}=0 \quad (7)$$

here μ_F - the Fermi gas chemical potential, $I(y)$ - ionization potential, which is appear in the equation as a smoothing spline by the experimental stages of ionization values - $I(1)$, $I(2)$ etc. $B(V,T_e)$ is used to take into account cold ionization of compressed matter and b, β, σ, μ - parameters, which are constructed using shock compression experimental data for metals.

For the describing free energy we use approximation of an ideal Fermi gas:

$$F_e=yT_e\left(\frac{3}{5}\varphi-\frac{3}{2}\ln\left(1+\frac{5}{2\varphi}\right)\right) \quad (8)$$

Second part F_i is linked to the transition from states at different temperatures:

$$F_i=\frac{3}{2}T_i ln\frac{1+\lambda G}{V^{\frac{2}{3}}T} \quad (9)$$

where $G=(\frac{4\pi}{3})^{\frac{1}{3}}\frac{{y_c}^2(V)}{V^{\frac{1}{3}}T_i}$ and $y_c(V)$ is a function of the cell volume V, which is defined by the ionization equation. Using Helmholtz free energy we receive necessary formulas for the pressure of the electrons and the internal energy:

$$P_e=\frac{1}{5}(3\pi^2)^{\frac{2}{3}}(\frac{y}{V})^{\frac{5}{3}}+T_e(\frac{y}{V})\left(1+\frac{2}{5}\varphi\right)^{-1} \quad (10)$$

$$\varepsilon_e=\frac{3}{2}VP \quad (11)$$

$$P_i=\frac{T_i}{V}\frac{1+3\lambda(\frac{1}{2}-\frac{dlny_c(V)}{dlnV})G}{1+\lambda \mathrm{G}} \quad (12)$$

$$\varepsilon_i=\frac{3}{2}T_i\frac{1+2\lambda \mathrm{G}}{1+\lambda \mathrm{G}} \quad (13)$$

And finally, in P_{ei} we consider that it should not have an influence on the equation of ionization, total pressure at normal density and zero temperature must be equal zero, at a fixed density interaction between electrons and ions should decrease as the temperature increases, at low densities it must decrease fast:

$$P_{ei}=-\frac{1}{5}(3\pi^2)^{\frac{2}{3}}(\frac{y_0}{V_0})^{\frac{5}{3}}(\frac{V_0}{V})^{\frac{4}{3}}\frac{1+\delta}{1+[\delta+(1+\delta)T_e/T^*](\frac{V}{V_0})^{\gamma}} \quad (14)$$

where V_0, γ, δ, T^* are the parameters, which can be configured using values of the density, of the sublimation energy, of the isothermal compressibility and of the metal thermal expansion coefficient.

3. Results

To verify our mathematical model, the ablation depth for aluminum and copper is calculated and compared with the experiment. This experimental data is collected for an average depth of machined grooves after using laser pulses with 170 fs duration. In Figure 2 the computer simulation results are shown, and they are in well agreement for various laser fluence values.

For copper we also compare results with experiment values of ablation depth for different values of the laser fluence which are received for the single laser shots and machined grooves by multiple laser pulses with 100 fs duration with same total energy (Figure 3).

For a single pulse computer simulation results well match with experimental values, but we also receive a good agreement for a data in other case. Some differences can be explained by the fact that the experimental ablation depth per pulse for them is estimated in the way that the measured groove depth is divided by the number of laser shots. This multi pulse laser radiation in the same spot may lead to the changes in the surface optical properties because of increasing roughness. Furthermore, inclined groove walls in the case of deep groves could significantly change the reflection of a laser beam. Some investigations of these problems are needed, and the results may be included in this model later.

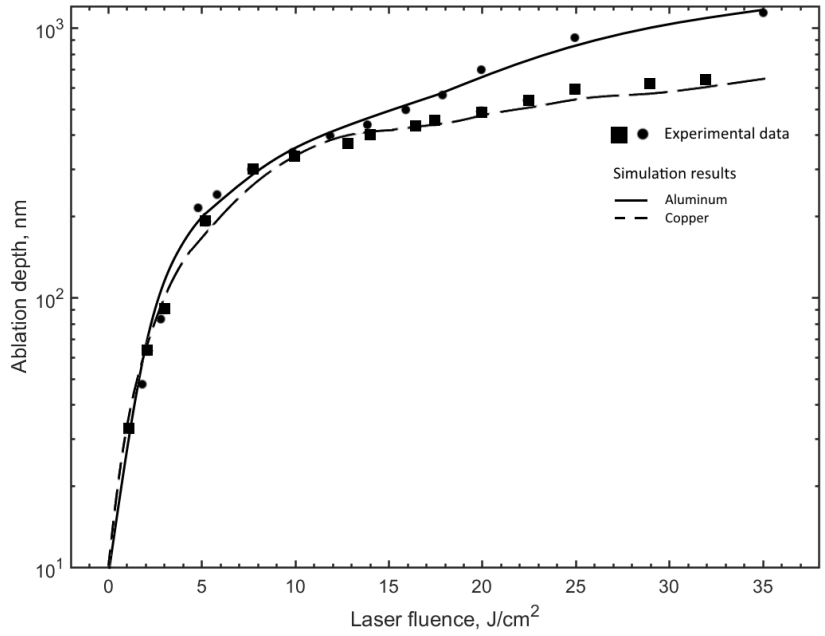

Figure 2. Experimental and numerically calculated ablation depth for aluminum and copper.

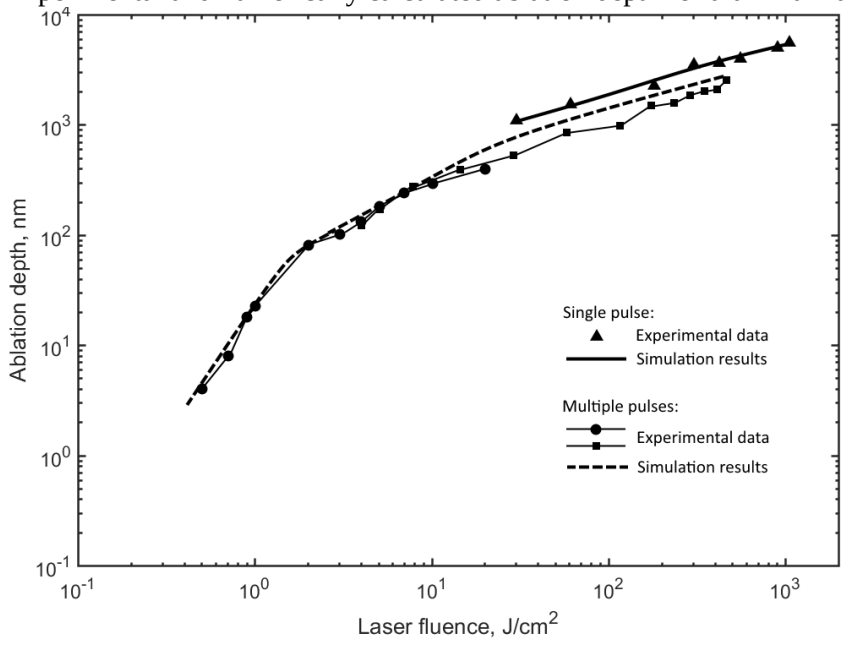

Figure 3. Experimental and numerically calculated ablation depth for copper.

4. Conclusions

In this article a mathematical model for laser ablation of metals by femtosecond duration laser pulses is developed. A wide-range equation of state for metals is used to increase the accuracy of calculations. The numerical results for metals are compared with experimental data for ablation depth at different laser fluence and duration of pulses. The results for both metals are in a good agreement with the experiment.

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