Computer modelling of pulsed laser femtosecond ablation for metals

R V Davydov, V I Antonov
Peter the Great St.Petersburg Polytechnic University, Saint Petersburg, Russia

E-mail: davydovroman@outlook.com

Abstract. In this article a mathematical model for a femtosecond pulsed laser ablation for metals is proposed. This model is based on two-temperature model for electrons and ions with addition of hydrodynamic part and wide-range semi-empirical equation of state for metals. The results of the modelling for several metals are compared with experimental data at different laser fluence and duration of pulses for ablation depth. A good agreement with them and the experiment is received.

1. Introduction
Laser material processing by femtosecond duration pulses is demonstrated nowadays as an effective way for micro/nano machining [1], surface structural modification [2] and material removal of solid materials (ablation) [3] by reason of its minimal heat affected zone and well reproducibility. Ultra short laser pulse ends before the expanding of plasma occurs, leading to improved efficiency as the laser energy is absorbed at the interface of the material rather than in the generated plasma. One more advantage of femtosecond laser ablation is that the use of ultra short laser pulses enables the deposition of energy and removal of a thin layer in time scales much faster than required for transferring the energy into the main part of the material. For metals, it happens because the finite heat conduction time, for dielectrics the removal take place on a time scale faster comparing to the electron-phonon coupling [4]. Based on this, femtosecond laser ablation proceed with small secondary damage to the surrounding material, in opposite to nano-or pico- laser ablation [5].

Despite a lot of research work, it is still difficult to make an accurate prediction of ablation processes, because they are significantly depending on laser parameters, target material characteristics and the surrounding medium [6-8]. For computer simulation of laser ablation, there are two main approaches are used now - molecular dynamic models and continuous thermodynamic models. In the molecular dynamic models trajectories (positions and velocities) are found by numerical solution of the equations of motion for all atoms in the system with the use of chosen interatomic interaction potential that defines the equilibrium structure and thermodynamic properties of the material [9]. The main advantage of this technique is that no further assumptions on the processes are required for it, 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 [10]. In thermodynamic approach a two-temperature model is widely employed for the simulation of ultra-short laser processing [11]. This continuous model describes the energy transfer inside a metal with two coupled generalized heat conduction equations for the temperatures of the electrons and the lattice. To describe the material removal processes this model can be used together with a system of hydrodynamic equations. However, when interaction between material
and laser radiation is studied, an appropriate description of the thermodynamic properties of matter is required over a broad region of states including plasma at high pressures and temperatures and normal conditions. So the choice of an equation of state, required for solving the hydrodynamic equations, can significantly affect the results [12].

Therefore, there is still a need to develop a mathematical model with which computer simulation of laser ablation can be conducted at various parameters enough quickly and accurately. In our work we propose a mathematical model which is based on two-temperature model with developed wide-range equation of state for receiving better accuracy.

2. Mathematical model

In this article we propose a model in a two-temperature form according to conservation laws of mass, momentum and energy of electron and ion subparts:

\[ \frac{\partial}{\partial t} \left( \frac{1}{\rho} \right) + \frac{\partial \rho \dot{v}}{\partial m} = 0 \]  
\[ \frac{\partial \rho \dot{v}}{\partial t} \frac{\partial \rho \dot{p}}{\partial m} = 0 \]  
\[ \frac{\partial \rho \dot{v}}{\partial t} + P_e \frac{\partial \rho \dot{v}}{\partial m} = - \frac{a_{ei}}{\rho} (T_e - T_i) + \frac{\partial}{\partial m} \left( k \rho \frac{\partial T}{\partial m} \right) + I_L \]  
\[ \frac{\partial \rho \dot{e}_e}{\partial t} + P_e \frac{\partial \rho \dot{e}_e}{\partial m} = a_{ei} (T_e - T_i) \]

where \( m \) is the mass coordinate, \( dm = p \, dX, m = \int_{x_0}^{x} p \, dX \), direction of \( x \)-axis is chosen perpendicular to the surface of the metal, \( \dot{v} \) is the velocity, \( t \) is the time, \( \rho \) and \( \rho_0 \) are the density and the initial density, \( T_e \) and \( T_i \), \( \varepsilon_e \) and \( \varepsilon_i \), \( P_e \) and \( P_i \) are the temperatures, internal energies and the pressures of electrons and ions, \( P = P_e + P_i \) and \( \varepsilon = \varepsilon_e + \varepsilon_i \) are the full pressure and the internal energy, \( a_{ei} \) - coefficient of electron-ion relaxation [13], \( J_L \) - energy of the absorbed laser radiation, described by:

\[ I_L = \frac{B}{\tau_0 \sqrt{\pi} \delta} \exp \left( \frac{x(m, t) - x(m, \bar{t})}{\delta} \right) \exp \left( - \frac{t_0^2}{\tau_0^2} \right) \]

Here \( B \) is the laser radiation energy, \( \tau_0 \) is the laser pulse duration, \( \delta \) is the skin depth of metal.

To solve the system of hydrodynamic equations in the two-temperature model we use wide-range semi-empirical two-temperature equation of state [14]. The solution of the system of equations is carried out by iteration method with splitting into physical processes, we consider separately the hydrodynamic motion of matter upon absorption of laser radiation, electronic thermal conductivity, and energy exchange between electrons and ions. At the first step we take into account only the hydrodynamics and the absorption of the laser radiation by the substance. For approximation we use fully conservative finite-difference scheme, which was described by Samarskii [15] and modified for two-temperature situation. Oscillations arising in the calculation of solutions with discontinuities are corrected by introducing an artificial viscosity. At the second step, the process of heat transfer by electrons is considered and the one-dimensional nonlinear heat conduction equation is solved. And at the third step we solve system of ordinary differential equations for electron-ion exchange.

3. Results and discussion

To verify our mathematical model, the ablation depth for copper and aluminum is calculated and compared with the experimental data for an average depth of machined grooves after using laser pulses with 170 fs duration. As we can see in Figure 1 and Figure 2 simulation results are close to experimental data for both metals at various laser fluence values.
Figure 1. Experimental and calculated ablation depth for copper.

Figure 2. Experimental and calculated ablation depth for aluminum.

For copper we also compare results with experimental data for a wide range of laser fluence (up to 1037 J/cm²), which are received for single laser shots and machined grooves by multiple laser pulses with 100 fs duration (Figure 3).
Figure 3. Experimental and calculated ablation depth for copper.

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

4. Conclusion
In this article a mathematical model for laser ablation of metals by femtosecond 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.

References
[1] Chen F, Aldana J R 2014 Laser & Photonics Reviews 28(2) 251–275
[2] Bonse J, Koter R, Hartelt M, Spaltmann D, Pentzien S, Hohm S, Rosenfeld A, Kruger J 2014 Applied Physics A. 117(1) 103–110
[3] Zeng H, Du X W, Singh S C, Kulinich S A, Yang S, He J, Cai W 2012 Advanced Functional Materials 22(7) 1333
[4] Balling P, Schou J 2013 Reports on Progress in Physics 76(3) 036502
[5] Ionin A A, Kudryashov S I, Samokhin A A 2017 Phys. Usp. 60 149–160
[6] Myazin N S, Smirnov K J, Davydov V V, Logunov S E 2017 J. Phys.: Conf. Ser. 929(1) 012064
[7] Smirnov K J, Medzakovskiy V I, Davydov V V, Vysoczky M G, Glagolev S F 2017 J. Phys.: Conf. Ser. 917(6) 062019
[8] Vologdin V A, Davydov V V, Velichko E N 2016 J. Phys.: Conf. Ser. 741(1) 012095
[9] Ivanov D S, Lipp V P, Veiko V P, Yakovlev E, Rethfeld B 2014 Applied Physics A 117(4) 2133
[10] Wu C, Zhigilei L V 2014 *Applied Physics A* **114**(1) 11
[11] Ren Y, Cheng C W, Chen J K, Zhang Y, Tzou D Y. 2013 *International Journal of Thermal Sciences* **70** 32
[12] Cheng C W, Wang S Y, Chang K P, Chen J K 2016 *Applied Surface Science* **361** 41
[13] Davydov R V, Antonov V I 2016 *J. Phys.: Conf. Ser.* **769**(1) 012060
[14] Davydov R V, Antonov V I 2017 *J. Phys.: Conf. Ser.* **929**(1) 012040
[15] Samarskii A A, Popov Yu P 1992 *Difference schemes for gas dynamics* (Moscow: Nauka)