Numerical analysis of laser ablation using the axisymmetric two-temperature model

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Abstract

Laser ablation of the axisymmetric micro-domain is analyzed. To describe the thermal processes occurring in the micro-domain the two-temperature hyperbolic model supplemented by the boundary and initial conditions is used. This model takes into account the phase changes of material (solid-liquid and liquid-vapour) and the ablation process. At the stage of numerical computations the finite difference method with staggered grid is used. In the final part the results of computations are shown.

Keywords: laser heating, phase changes, two-temperature model, melting, evaporation, ablation, finite difference method

1. Introduction

The ablation of the axisymmetric micro-domain subjected to the ultra-short laser pulse is considered. Two-temperature hyperbolic model with nonlinear physical parameters is used. This model consists of equations describing the temporal and spatial evolution of the lattice and electrons temperatures, lattice and electron heat fluxes and also the isothermal solid-liquid (or liquid-vapour) phase change. The algorithm based on the explicit scheme of the finite difference method with the staggered grid is proposed. In the final part the results concerning the ablation process are presented.

2. Governing equations

Axisymmetric domain exposed to the ultra-short laser pulse is considered. Two-temperature model describing the temporal and spatial evolution of the lattice and electrons temperatures is of the form [1]

$$\begin{aligned} C_e(T_e)\frac{\partial T_e}{\partial t} &= -\nabla\cdot\mathbf{q}_e - G(T_e,T_l)\left(T_e-T_l\right)+Q(r,z,t) \\ C_l\frac{\partial T_l}{\partial t} &= -\nabla\cdot\mathbf{q}_l + G(T_e,T_l)\left(T_e-T_l\right)+Q_m(r,z,t)+Q_{ev}(r,z,t) \end{aligned} \tag{1}$$

where $T_e = T_e\,(r, z, t)$, $T_l = T_l\,(r, z, t)$, $\mathbf{q}_e = \mathbf{q}_e\,(r, z, t)$, $\mathbf{q}_l = \mathbf{q}_l\,(r, z, t)$ are the temperatures and heat fluxes of the electrons and lattice, respectively, $C_e(T_e)$, C_l are the volumetric specific heats, $G(T_e, T_l)$ is the electron-phonon coupling factor, $Q(r, z, t)$ is the source function associated with the irradiation, while $Q_m(r, z, t)$ and $Q_{ev}\,(r, z, t)$ are the source functions associated with the melting and evaporation, respectively. For low laser intensity, when the lattice temperature does not exceed the melting point the functions $Q_m\,(r, z, t)$ and $Q_{ev}\,(r, z, t)$ are equal to zero, of course.

Between the heat fluxes and temperature gradients the following formulas are introduced

$$\mathbf{q}_e+\tau_e\frac{\partial\mathbf{q}_e}{\partial t}=-\lambda_e(T_e,T_l)\nabla T_e,\quad \mathbf{q}_l+\tau_l\frac{\partial\mathbf{q}_l}{\partial t}=-\lambda_l\nabla T_l \tag{2}$$

where $\lambda_e = \lambda_e(T_e, T_l)$, λ_l are the thermal conductivities of the electrons and lattice, respectively, τ_e is the relaxation time of free electrons in metals, τ_l is the relaxation time in phonon collisions and $\nabla(\cdot)$ denotes the gradient.

It should be noted that for high laser intensity the volumetric specific heat and thermal conductivity of electrons as well as the coupling factor are temperature-dependent functions [1, 2].

The laser irradiation is described by a source term introduced in the equation (1) [3]

$$Q=\sqrt{\frac{4\ln 2}{\pi}}\left(1-R\right)\frac{I_0}{\delta t_p}\exp\left[-\frac{r^2}{r_D^2}-\frac{z}{\delta}-4\ln 2\frac{\left(t-2t_p\right)^2}{t_p^2}\right] \tag{3}$$

where I_0 is the laser intensity, t_p is the characteristic time of laser pulse, δ is the optical penetration depth, R is the reflectivity of the irradiated surface and r_D is the laser beam radius.

The internal heat sources resulting from the phase changes (melting and evaporation) take a form

$$Q_m(r,z,t)=-L_m\frac{\partial S_m(r,z,t)}{\partial t},\quad Q_{ev}(r,z,t)=-L_{ev}\frac{\partial S_{ev}(r,z,t)}{\partial t} \tag{4}$$

where L_m is the volumetric heat of fusion, L_{ev} is the volumetric heat of evaporation, S_m and S_{ev} are the volumetric molten and gaseous state fractions in the surroundings of the point considered. Both S_m and S_{ev} are equal to zero at the beginning of heating process and increase from 0 to 1 when the local temperature achieves the melting T_m and boiling T_{ev} temperatures, respectively.

The ablation effect is modeled in this way that when at the point considered the value S_{ev} exceeds 1 then the sub-domain corresponding to this point is removed, while the appropriate boundary conditions are transferred to the new external boundary.

The above presented mathematical model is supplemented by the boundary conditions (no-flux conditions), it means

$$(r,z)\in\Gamma:\quad \begin{aligned} q_{be}\left(r,z,t\right)&=-\lambda_e(T_e,T_l)\,\mathbf{n}\cdot\nabla T_e(r,z,t)=0 \\ q_{bl}\left(r,z,t\right)&=-\lambda_l\,\mathbf{n}\cdot\nabla T_l(r,z,t)=0 \end{aligned} \tag{5}$$

where $\mathbf{n}$ is the outward unit normal vector.

The initial temperature distribution is also known

$$t=0:\quad T_e\left(r,z,t\right)=T_l\left(r,z,t\right)=T_0 \tag{6}$$

where T_0 is constant.

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3. Method of solution and results of computations

In the cylindrical coordinate system

$$\nabla \cdot \mathbf{q}(r, z, t) = \frac{1}{r}\frac{\partial (r q_r)}{\partial r} + \frac{\partial q_z}{\partial z} \tag{7}$$

and then the equations (1), (2) take a form

$$C_e(T_e)\frac{\partial T_e(r,z,t)}{\partial t} = -\frac{1}{r}\frac{\partial\left[r q_{e\,r}(r,z,t)\right]}{\partial r} - \frac{\partial q_{e\,z}(r,z,t)}{\partial z} - G(T_e, T_l)\left[T_e(r,z,t) - T_l(r,z,t)\right] + Q(r,z,t) \tag{8}$$

$$C_l(T_l)\frac{\partial T_l(r,z,t)}{\partial t} = -\frac{1}{r}\frac{\partial\left[r q_{l\,r}(r,z,t)\right]}{\partial r} - \frac{\partial q_{l\,z}(r,z,t)}{\partial z} + G(T_e, T_l)\left[T_e(r,z,t) - T_l(r,z,t)\right] + Q_m(r,z,t) + Q_{ev}(r,z,t) \tag{9}$$

$$\begin{aligned} q_{er} + \tau_e\frac{\partial q_{er}}{\partial t} &= -\lambda_e(T_e, T_l)\frac{\partial T_e}{\partial r}, \quad q_{l\,r} + \tau_l\frac{\partial q_{l\,r}}{\partial t} = -\lambda_l(T_l)\frac{\partial T_l}{\partial r} \\ q_{ez} + \tau_e\frac{\partial q_{ez}}{\partial t} &= -\lambda_e(T_e, T_l)\frac{\partial T_e}{\partial z}, \quad q_{l\,z} + \tau_l\frac{\partial q_{l\,z}}{\partial t} = -\lambda_l(T_l)\frac{\partial T_l}{\partial z} \end{aligned} \tag{10}$$

To solve the equations (7) – (10) the explicit scheme of finite difference method with the staggered grid, as shown in Figure 1, is used. The details of the algorithm will be presented in the full version of the paper.

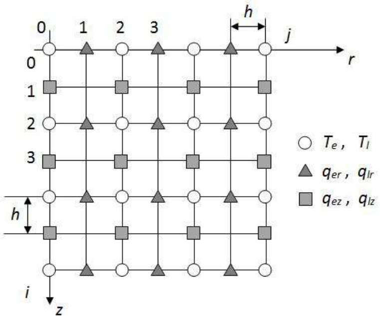

Figure 1: Staggered grid

When the local lattice temperature $T_{lij}{}^f$ at the node (r_i, z_j) and at the moment of time t^f achieves the value of melting point T_m ($T_{lij}{}^f \geq T_m$) then in the sub-domain $r \in [r_{i,j-1}, r_{i,j+1}]$, $z \in [z_{i-1,j}, z_{i+1,j}]$ the melting process starts. It is assumed that the melting process proceeds at the constant temperature and then the left-hand side of equation (9) is equal to zero. Using the dependence (4) the appropriate difference equation which determines the value $S_{m\,i\,j}{}^f$ can be derived. When the function $S_{m\,i\,j}{}^f$ reaches the value 1 then the melting process is finished and the calculations are performed based on equation (9) under the assumption that $Q_m = Q_{ev} = 0$. Next, when the local lattice temperature $T_{lij}{}^f$ achieves the value of boiling point T_{ev} then using the dependence (4) the value $S_{ev\,i\,j}{}^f$ (in a similar way as in the case of melting) can be calculated. Finally, when the function $S_{ev\,i\,j}{}^f$ reaches the value 1 then the sub-domain considered is removed, while the appropriate boundary conditions were transferred to the new external boundary.

The cylindrical domain (R = $100\cdot10^{-9}$ m, Z = $100\cdot10^{-9}$ m) of the initial temperature T_p = 300 K subjected to the short-pulse laser heating is considered. Thermophysical parameters for gold are taken from [1, 2].

The laser beam radius is equal to $r_D = R/8$. To observe heating, melting, evaporation and ablation process the value of laser intensity $I_0 = 1.5\cdot10^6$ J/m^2 is assumed and the characteristic time of laser pulse is equal to t_p =100 ps. Calculations are made for 50×50 = 2500 (h = 2 nm) 'temperature nodes', time step is equal to 0.001 ps.
Figure 2 presents the domain with ablated part (color black) for two different moments of time, namely 300 ps and 400 ps.

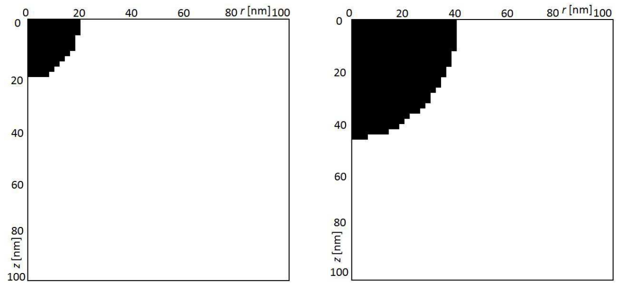

Figure 2: Domain with ablated part at the moments of time 300 ps and 400 ps

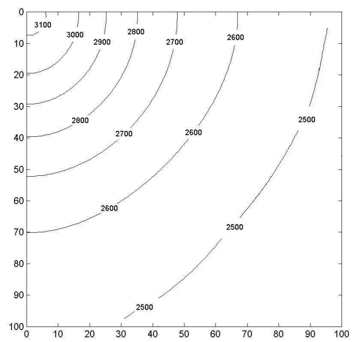

Figure 3: Temperature distribution for time equals 250 ps

4. Conclusions

Numerical model of melting, evaporation and ablation processes proceeding in the domain subjected to the laser heating is presented. In should be noted that depending on the laser power only the melting process or only the heating process in the domain considered can be observed.

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References

[1] Chen, J. K., Tzou, D. Y., Beraun, J. E. A semiclassical two-temperature model for ultrafast laser heating. *Int J Heat Mass Transf*, 49, pp. 307-316, 2006.

[2] Majchrzak, E., Dziatkiewicz, J., Analysis of ultashort laser pulse interactions with metal films using a two-temperature model, *J. Appl. Math. Comput. Mech.*, 14(2), pp. 31-39, 2015.

[3] Grigoropoulos, C. P.; Chimmalgi, A.; Hwang, D.J. Nano-structuring using pulsed laser radiation. *Laser Ablation and its Applications, Springer Series in Optical Sciences*, 129, 473-504, 2007.