Numerical Simulation and Analysis on 3D Temperature Field of the Metal Ablated with Femtosecond Pulse Laser

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Abstract. To describe femtosecond laser ablation on the metal, numerical simulation on the basis of the double-temperature equation for three-dimension temperature field of the copper ablated with femtosecond pulse laser was performed by finite-difference method. Based on imbalance of the electronic and lattice’s temperatures, the calefactive process of the electron and the lattice was obtained, respectively. The dependence of the electron-lattice coupling time on irradiated laser fluence was studied. The ablation depth and the ablation radius of the copper for single pulse fluence were calculated. The dependence of the start ablation (phase explosion arises) time of the copper on irradiated laser fluence was studied. The results indicate that the material jet due to phase explosion is earlier and the duration of ablation is longer with the increase of the laser fluence. When the laser fluence is higher than 1.5J/cm², the ablation start time is about 2-3 ps.

1. Introduction

In recent years, femtosecond pulsed laser have shown great potential in the micro-nano machining field. Many issues group and researchers made a lot of research results in this area. Research on the interaction of ultrashort intense laser and materials had been attended more and more by the research scholars [1-3]. Femtosecond laser ablation on the materials is a fast and complex process. For understanding the properties and accumulating theoretical basis of femtosecond laser ablate the material, investigate on the temperature field of the material ablated with femtosecond pulse laser is a important issue. The double-temperatures model for metal was first established by the Soviet scholars S.I.Anisimov et al according to the non-steady state heat conduction equation [4]. The electronic and the lattice are divided into two systems in the model. And the temperature changes of the electronic and the lattice were described respectively. The model was built on the basis of reasonable physical analysis. And scholars have a series theoretical and experimental research on the interaction of ultra short intense laser and metal by one-dimensional double-temperature equation (DTE) [2,3,5-8]. The heat affected zone had been simulated when a rectangular pulse laser ablate the aluminium by French scholar S. Valette et al used the DTE and finite difference method (FDM) [9]. The numerical result was consistent with the literature [10].

In this paper, we report numerical simulation for 3D temperature field of the metal ablated with femtosecond pulse laser by the DTE and FDM. Based on imbalance of the electronic and the lattice
temperatures, the calefactive process of the electron and lattice was obtained, respectively. The dependence of the electron-lattice energy coupling time on irradiated laser pulse energy was studied. The threshold fluence of single pulse in the copper had been obtained. The ablation depth and radius of the copper for single pulse fluence were calculated. The dependence of the start ablation (phase explosion arises) time of the copper on irradiated laser pulse fluence was studied.

2. Theoretical model
For the metal material, when the laser pulse duration was shorter than the electron-lattice energy coupling time, the time evolution of the electron and lattice temperatures can be described by two coupled nonlinear differential equation, i.e. the double-temperature equation:

\[
C_e \frac{\partial T_e}{\partial t} = \nabla (K_e \nabla T_e) - g(T_e - T_i) + S
\]

\[
C_i \frac{\partial T_i}{\partial t} = g(T_e - T_i)
\]

In these equations, \(C_e\) and \(C_i\) are the specific heats of the electron and lattice, respectively. \(T_e\) and \(T_i\) are the electron and lattice temperatures, respectively. \(K_e\) is the electron thermal conductivity. \(g\) is electron-lattice coupling coefficient. \(C_e\) and \(K_e\) vary with the changing electron temperature: \(C_e = C_e' T_e, \quad K_e = K_e' T_e / T_i\). \(S\) is the laser source items and is written as follows:

\[
S(z, r, t) = I_0 \alpha (1 - R) \exp[-4\ln2\left(\frac{t}{T_0}\right)^2] \exp[-\left(\frac{r}{r_0}\right)^2] \exp(-\alpha z)
\]

Where: \(z\) is the laser direction. The laser direction is perpendicular to the material surface. \(r\) is the radius direction of laser beam. \(r_0\) is the radius of the laser beam at the focusing point. \(R\) is the reflectance of the material surface. \(\alpha\) is the absorption coefficient of the material. \(I_0\) is the peak power. \(T_0\) is the laser pulse duration.

3. Results and discussions
In the present work, it is assumed that the material is a half of infinity, \(T_0=150fs, \quad r_0=8\mu m,\) the initial temperatures of the electron and lattice both are 300K. Table 1 gives all the numerical data used to the system in the case of a copper sample.

| metal | \(g\) (Wm\(^{-3}\)K\(^{-1}\)) | \(C_e'\) (Jm\(^{-3}\)K\(^{-2}\)) | \(K_{\phi0}\) (Wm\(^{-1}\)K\(^{-1}\)) | \(C_i'\) (Jm\(^{-3}\)K\(^{-1}\)) | \(R\) | \(\alpha\) (/nm) | \(T_0\) (K) |
|-------|-----------------|-----------------|-----------------|-----------------|--------|--------|---------|
| Cu    | 12x10\(^{-6}\)  | 96.6            | 401             | 3.43x10\(^7\)  | 0.329  | 0.089  | 5890    |

To describe femtosecond laser ablation on the copper, numerical simulation on the basis of the DTE for 3D temperature field of the copper ablated with femtosecond pulse laser is performed by FDM. Based on imbalance of the electronic and the lattice’s temperature, the calefactive process of the electron and the lattice was obtained, respectively. To femtosecond laser, the ablation of the material mainly is caused by phase explosion [11-13]. Because the energy injection time is very short, leading to that no time to spread, the temperature of the irradiated material rises rapidly, until the temperature of the material reached to 0.9\(T_c\) (\(T_c\) is the thermal dynamic equilibrium critical temperature), and then it is ejected from the metal surface. Therefore, in this simulation, the metal material can be ablated when the lattice’s temperature is increased to 0.9\(T_c\).
Figure 1 represents the evolution of the temperature of the electron and lattice with different incident laser pulse fluence. It can be observed that the electron temperature rises rapidly to the maximum and the lattice temperature keeps fixed in the duration of the femtosecond laser. After the laser pulse finishes, the electron-lattice energies exchange start off and the lattice temperature rises. The electron-lattice energy coupling time is relative to the incident laser fluence. As the laser fluence is greater, the electron-lattice energy coupling time goes into longer and the lattice temperature goes into higher after coupling. The incident fluence that makes the equilibrium temperature of the electron and lattice in accord with critical temperature is called the threshold fluence. When the laser fluence is increased to the threshold fluence, the center of material was ablated justly. The threshold fluence of single pulse in the copper is 0.76J/cm$^2$ by calculations, which is approximately consistent with the literature [14] (In the literature [14], the threshold fluence is 0.7 J/cm$^2$). And electron-lattice coupling time by calculations is about 17.06ps, accordingly.

Figure 1. The time evolution of electron and lattice temperatures in the surface layer center of the copper with different incident laser pulse energies.

Figure 2 represents the change of the electron-lattice energy coupling time in the center of copper surface versus the single pulse fluence. It can be seen that the electron-lattice energy coupling time is nearly relative to the incident fluence when it is below the threshold fluence. The electron-lattice energy coupling time becomes longer with the increasing laser fluence. When the incident fluence increases to the threshold fluence, the coupling time reaches maximum.

Figure 2. The change of the electron-lattice energy coupling time in the surface layer center of copper versus the pulse fluence.

Figure 3. The change of the ablation start (phase explosion arises) time versus the laser energy for copper. The so-called the ablation start time of the metal material, that is the time that the lattice’s temperature is increased to 0.9$T_c$ and then the material is ejected from the metal surface. From Figure 3, it can be seen that the higher laser pulse fluence, the earlier ablation start time. When the laser fluence is higher than 1.5 J/cm$^2$, the ablation start time is about 2-3 ps. With the further increasing laser fluence, the ablation start time finally becomes changeless.
Figure 4. Lattice temperature evolution for propagation direction of the beam, leading to an estimation of the ablated depth with different single pulse fluence for copper.

Figure 5. Lattice temperature evolution for radial direction of the beam, leading to an estimation of the ablated radius with different single pulse fluence for copper.

Figure 4 represents the lattice temperature evolution for propagation direction of the beam, leading to an estimation of the ablated depth. Figure 5 represents the lattice temperature evolution for radial direction of the beam, leading to an estimation of the ablated radius. From Figure 4 and 5, we can see that the ablation velocity and the thermal effects zone relatively are larger when the ablation fluence is higher in the copper. The ablation in the copper can be mainly finished in 15-20 ps. The numerical results also show that the ablation depth and radius are gradually increasing along with the increase of the laser fluence and finally become changeless. It can be due to the injection depth and spot size of incident laser.

4. Summary
In short, we have reported numerical simulation for 3D temperature field of the metal ablated with femtosecond pulse laser by the DTE and FDM. The threshold fluence of single pulse in the copper had been obtained. The numerical results show that the electron-lattice energy coupling time presents a steady increase with the increase of the laser fluence. The copper jet due to phase explosion is earlier and the duration of ablation is longer with the increase of pulse fluence. When the laser fluence is higher than 1.5 J/cm$^2$, the ablation start time is about 2-3 ps. With the further increasing laser fluence, the ablation start time finally becomes changeless. The ablation velocity and the thermal effects zone relatively are larger when the ablation fluence is higher in the copper. The ablation in the copper can be mainly finished in 15-20 ps.

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