www.czasopisma.pan.pl PAN www.journals.pan.pl

ARCHIVES
of
FOUNDRY ENGINEERING

DOI: 10.2478/v10266-012-0115-9

Published quarterly as the organ of the Foundry Commission of the Polish Academy of Sciences

ISSN (2299-2944)
Volume 12
Issue 4/2012

105 – 108

Numerical Modeling of Melting Process of Thin Metal Films Subjected to the Short Laser Pulse

E. Majchrzak*, J. Dziatkiewicz
Institute of Mechanics and Computational Engineering, Silesian University of Technology, Konarskiego, 44-100 Gliwice, Poland
*Corresponding author. E-mail address: ewa.majchrzak@polsl.pl

Received 02.07.2012; accepted in revised form 03.09.2012

Abstract

Thin metal film subjected to a short-pulse laser heating is considered. The parabolic two-temperature model describing the temporal and spatial evolution of the lattice and electrons temperatures is discussed and the melting process of thin layer is taken into account. At the stage of numerical computations the finite difference method is used. In the final part of the paper the examples of computations are shown.

Keywords: Application of Information Technology to the Foundry Industry, Numerical Techniques, Micro-Scale Heat Transfer, Melting process, Finite Difference Method

1. Introduction

Phase changes often occur in laser material processing. The interaction of the laser beam and metal can cause the rise of surface temperature above melting point and partial melting of layer. When the duration of laser pulse is around 10^{-13} s, which is the mean free time between collisions of electrons in metals, nonequilibrium between electrons and the lattice is significant and can't be analyzed using the classical heat transfer models [1, 2, 3]. In this case the two-temperature model is accepted for simulating femtosecond laser-material interactions [2, 3, 4, 5, 6].

In this paper the thin metal film subjected to the ultra-short laser pulse is considered. The problem is described by two coupled parabolic equations determining the electron and lattice temperatures. Laser action is taken into account in the internal source function appearing in the equation concerning the electron temperature. The melting model basing on the one domain method [7, 8, 9] widely used in macroscopic heat transfer is proposed. The problem is solved by means of the explicit scheme of finite difference method. In the final part of the paper the results of computations are shown and the conclusions are formulated.

2. Formulation of the problem

The thin metal film of thickness L (1D problem) subjected to the laser pulse is considered. Electrons temperature is described by the following equation

$$C_e(T_e)\frac{\partial T_e(x,t)}{\partial t}=\frac{\partial}{\partial x}\left[\lambda_e(T_e,T_l)\frac{\partial T_e(x,t)}{\partial x}\right]-G(T_e,T_l)\left[T_e(x,t)-T_l(x,t)\right]+Q(x,t) \tag{1}$$

where T_e $(x,\ t)$, T_l $(x,\ t)$ are the temperatures of electrons and lattice, respectively, C_e (T_e) is the electrons thermal capacity,

$\lambda_e(T_e, T_l)$ is the electrons thermal conductivity, $G(T_e, T_l)$ is the electron-lattice coupling factor, Q is the laser source [4]

$$Q(x,t)=\sqrt{\frac{\beta}{\pi}}\frac{1-R}{t_p\,\delta}I_0\exp\left[-\frac{x}{\delta}-\beta\frac{(t-2t_p)^2}{t_p^2}\right] \tag{2}$$

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 $\beta = 4\ln(2)$ [4].

The lattice temperature in the liquid state $T_{l,l}$ and solid state $T_{l,s}$ is described by equations

$$C_{l,l}\frac{\partial T_{l,l}(x,t)}{\partial t}=\frac{\partial}{\partial x}\left[\lambda_{l,l}\frac{\partial T_{l,l}(x,t)}{\partial x}\right]+ G(T_e,T_l)\left[T_e(x,t)-T_{l,l}(x,t)\right] \tag{3}$$

and

$$C_{l,s}\frac{\partial T_{l,s}(x,t)}{\partial t}=\frac{\partial}{\partial x}\left[\lambda_{l,s}\frac{\partial T_{l,s}(x,t)}{\partial x}\right]+ G(T_e,T_l)\left[T_e(x,t)-T_{l,s}(x,t)\right] \tag{4}$$

where $C_{l,l}$, $C_{l,s}$, $\lambda_{l,l}$, $\lambda_{l,s}$ are the thermal capacities and thermal conductivities of lattice in the liquid and solid state, respectively.

At the solid-liquid interface $\xi(t)$ the Stefan boundary condition was assumed

$$x=\xi(t):\quad \begin{cases} T_{l,s}(x,t)=T_{l,l}(x,t)=T_m \\ \lambda_{l,s}\dfrac{\partial T_{l,s}(x,t)}{\partial x}-\lambda_{l,l}\dfrac{\partial T_{l,l}(x,t)}{\partial x}=Q_m u \end{cases} \tag{5}$$

where T_m is the melting point, Q_m is the volumetric latent heat of fusion, while $u = \mathrm{d}\xi(t)/\mathrm{d}t$ is the solid-liquid interfacial velocity.

Taking into account the short period of laser heating, heat losses from front and back surfaces of thin film can be neglected [4], this means

$$q_e(0,t)=q_e(L,t)=q_l(0,t)=q_l(L,t)=0 \tag{6}$$

where $q_e(x, t)$, $q_l(x, t)$ are the heat fluxes for electron and lattice systems, respectively.

The initial conditions are assumed to be constant

$$t=0:\quad T_e(x,0)=T_l(x,0)=T_p \tag{7}$$

3. Model of phase change

In this paper the following approach to the modeling of phase change in thin metal film is proposed. Instead of the melting temperature T_m the narrow interval temperature $[T_S, T_L]$ is introduced. In this interval of temperature the latent heat of fusion is emitted. In other words, the melting process in the constant temperature is substituted by melting process in the small interval of temperatures.

Then only one equation concerning the lattice is considered

$$C_l(T_l)\frac{\partial T_l(x,t)}{\partial t}=\frac{\partial}{\partial x}\left[\lambda_l(T_l)\frac{\partial T_l(x,t)}{\partial x}\right]+ G(T_e)\left[T_e(x,t)-T_l(x,t)\right]+Q_m\frac{\partial S(x,t)}{\partial t} \tag{8}$$

where $S(x, t)$ is the solid state fraction in the neighborhood of the point under consideration. Because

$$\frac{\partial S(x,t)}{\partial t}=\frac{\mathrm{d}S(T_l)}{\mathrm{d}T_l}\frac{\partial T_l(x,t)}{\partial t} \tag{9}$$

so the equation (8) can be written in the form

$$\left[C_l(T_l)-Q_m\frac{\mathrm{d}S(T_l)}{\mathrm{d}T_l}\right]\frac{\partial T_l(x,t)}{\partial t}= \frac{\partial}{\partial x}\left[\lambda_l(T_l)\frac{\partial T_l(x,t)}{\partial x}\right]+G(T_e)\left[T_e(x,t)-T_l(x,t)\right] \tag{10}$$

or

$$C(T_l)\frac{\partial T_l(x,t)}{\partial t}=\frac{\partial}{\partial x}\left[\lambda_l(T_l)\frac{\partial T_l(x,t)}{\partial x}\right]+ G(T_e)\left[T_e(x,t)-T_l(x,t)\right] \tag{11}$$

where

$$C(T_l)=C_l(T_l)-Q_m\frac{\mathrm{d}S(T_l)}{\mathrm{d}T_l} \tag{12}$$

is the so-called substitute thermal capacity of lattice. Because for $T_l < T_S$: $S(T_l) = 1$, this means $\mathrm{d}S(T_l)/\mathrm{d}T_l = 0$ and for $T_l > T_L$: $S(T_L) = 0$, this means $\mathrm{d}S(T_l)/\mathrm{d}T_l = 0$, the definition of substitute thermal capacity of lattice can be extended on the whole domain [7, 8, 9]. If one assumes that

$$T_S \le T_l \le T_L:\quad S(T_l)=\frac{T_l-T_L}{T_S-T_L} \tag{13}$$

and the thermal capacities of liquid and solid state are constant then the substitute thermal capacity of lattice is defined as follows (c.f. Figure 1)

$$C(T_l)=\begin{cases} C_L, & T_l > T_L \\ \dfrac{C_L+C_S}{2}+\dfrac{Q_m}{T_L-T_S}, & T_S \le T_l \le T_L \\ C_S, & T_l < T_S \end{cases} \tag{14}$$

Summing up, presented approach consists in the solution of equations (1), (11) supplemented by boundary conditions (6) and initial ones (7).

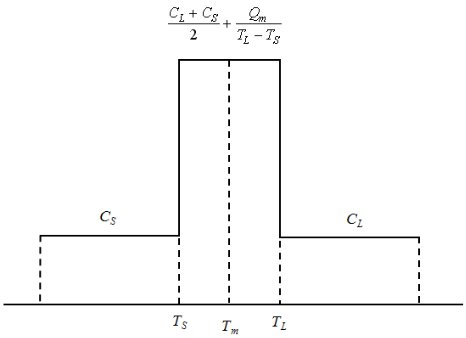

Fig. 1. Substitute thermal capacity of lattice

4. Examples of computations

The gold film of thickness L = 100 nm is considered. Initial temperature equals to T_p = 300 K. The layer is subjected to a short-pulse laser irradiation (R = 0.93, I_0 = 12000 J/m^2, t_p = 0.1 ps, δ =15.3 nm). The profiles of $C_e(T_e)$ and $G(T_e)$ are received from [10]. Thermophysical parameters for liquid and solid phase are the following: λ_l = 315 W/(mK), $C_L = C_S = 2.5 \cdot 10^6$ J/(m^3 K). The thermal conductivity of electrons $\lambda_e(T_e, T_l)$ was obtained from

$$\lambda_e(T_e,T_l) = D\, C_e(T_e)\frac{1}{AT_e^2 + BT_l} \tag{15}$$

where $A = 1.18 \cdot 10^7$ [1/(K^2·s)] i $B = 1.25 \cdot 10^{11}$ [1/(K·s)] [11] and

$$D = \frac{\hbar^2}{3m_e^2}\left(3\pi^2 n_e\right)^{\frac{2}{3}} \tag{16}$$

where h is the Planck constant divided by 2π (the Dirac constant), m_e is the effective mass of electrons, n_e is the number of electrons per unit of volume.

Melting temperature for thin gold film is equal to 1336K and the volumetric latent heat of fusion is equal to Q_m = 63730·19300 [J/m^3] [11]. The interval of melting temperature T_S = 1335K, T_L = 1337K is introduced.

The problem is solved using finite difference method [8] under the assumption that Δt = 0.0001 ps and h_x = 1 nm. Figure 2 shows the changes of electrons and lattice temperatures at the irradiated surface.

To estimate the influence of width of the melting temperature interval on the results of computations the error for electrons and lattice on the surface (x = 0) is calculated. This analysis is prepared for laser intensity I_0 = 6000 J/m^2. Other data are the same as previously.

The error for electrons and lattice was calculated from

$$Error_{e,0} = \frac{\sqrt{\frac{1}{F}\sum_{f=1}^{F}\left(T_{e,\pm 1K}^f - T_{e,\pm\Delta T}^f\right)^2}}{T_{e,\pm 1K\max}^f}\cdot 100\% \tag{17}$$

and

$$Error_{l,0} = \frac{\sqrt{\frac{1}{F}\sum_{f=1}^{F}\left(T_{l,\pm 1K}^f - T_{l,\pm\Delta T}^f\right)^2}}{T_{l,\pm 1K\max}^f}\cdot 100\% \tag{18}$$

where $T_{e,\pm 1K}^f$, $T_{l,\pm 1K}^f$ are the calculated electrons and lattice temperatures for the interval of melting [T_m – 1K, T_m + 1K], respectively, $T_{e,\pm 1K\max}^f$ is the maximum temperature for this melting interval and $T_{e,\pm\Delta T}^f$ is the temperature for increased width of melting temperature interval [T_S, T_L]. In table 1 the error analysis is presented.

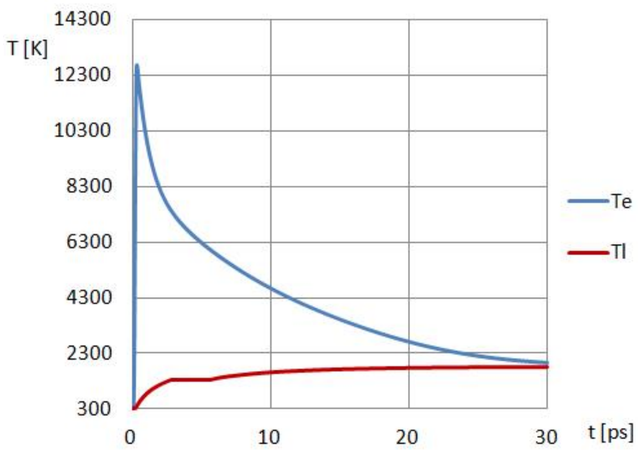

Fig. 2. Electrons and lattice temperature profiles on the irradiated surface – I_0 = 12000 J/m^2

Table 1.
Error analysis

The width of melting temperature interval [K]	Error for T_l [%]	Error for T_e [%]
1	1.289	0.031
10	1.806	0.030
20	2.348	0.036
50	2.513	0.048

As you can see this width changes have greater influence on lattice temperature. In figure 3 the lattice temperature profiles for different melting interval are shown. Additionally, in table 2 the maximum electrons and lattice temperature are shown.

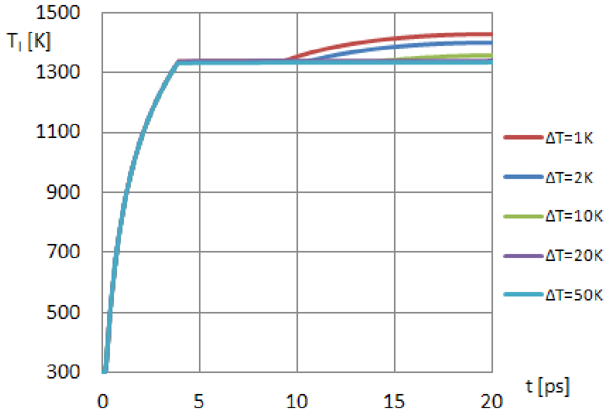

Fig. 3. Lattice temperature profiles on the irradiated surface for different melting interval – $I_0 = 6000$ J/m^2

Table 2.
Maximum electrons and lattice temperature for different width of melting interval

The width of melting temperature interval [K]	maximum T_l [K]	maximum T_e [K]
1	1426.372	13669.7179
2	1400.134	13669.7178
10	1358.981	13669.7177
20	1337.238	13669.7177
50	1333.760	13669.7176

5. Conclusions

Thin metal film subjected to the laser pulse has been considered. To describe the process analyzed the two-temperature parabolic model has been applied. The analysis of influence of the width of melting interval on electrons and lattice temperature is prepared.

It turned out that the changes of these parameters affected mainly on lattice temperature especially after exceeding the melting interval. It should be pointed out that narrow interval can neglect the melting process so it is important to choose it properly.

Acknowledgement

This work was funded by Grant No N N501 2167 37.

References

[1] Kannattey-Asibu, E. Jr.(2009). *Principles of laser materials processing*, New Yersey, John Wiley & Sons, Inc., Hoboken.
[2] Huang, J., Zhang, Y. & Chen J.K. (2009). Ultrafast solid-liquid-vapor phase change in a thin gold film irradiated by multiple femtosecond laser pulses. *International Journal of Heat and Mass Transfer*. 52, pp. 3091-3100.
[3] Anisimov, S.I., Kapeliovich, B.L. & Perel'man T.L. (1974). Electron emmision from metal surfaces exposed to ultrashort laser pulses. *Sov. Phys. JETP*. 39, 375-377.
[4] Chen, J.K. & Beraun, J.E. (2001). Numerical study of ultrashort laser pulse interactions with metal films. *Numerical Heat Transfer, Part A*. 40, 1-20.
[5] Qiu, T.Q. & Tien, C.L. (1994). Femtosecond laser heating of multi-layer metals - I Analysis. *Int. J. Heat Mass Transfer*. 37, 2789-2797.
[6] Majchrzak, E. & Poteralska, J. (2010). Numerical analysis of short-pulse laser interactions with this metal film. *Archives of Foundry Engineering*. 10 (4), 123-128.
[7] Mochnacki, B. & Suchy, J.S. (1995). *Numerical methods in computations of foundry processes*. Polish Foundrymen's Technical Association. Cracow.
[8] Mochnacki, B. (2011). In: Computational simulation and applications, Chapter 24: Numerical modeling of solidification process. Ed. Jianping Zhu, INTECH, 513-542.
[9] Mochnacki, B. & Szopa, R. (2011). Identification of alloy latent heat using the data of thermal and differential analysis. *Journal of Theoretical and Applied Mechanics*. 49 (4), 1019-1028.
[10] hppt://www.faculty.virginia.edu/CompMat/electron-phonon coupling/
[11] Christensen, B.H., Vestentoft, K. & Balling P. (2007). Short-pulse ablation rates and the two-temperature model. *Applied Surface Science*. 253, 6347-6352.