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Technical Note

Numerical simulation of laser-induced transient temperature field in film-substrate system by finite element method

B.Q. Xu [a,b], Z.H. Shen [b,*], J. Lu [b], X.W. Ni [b], S.Y. Zhang [c]

[a] Faculty of Science, Jiangsu University, Zhenjiang, Jiangsu 212013, People's Republic of China
[b] Department of Applied Physics, Nanjing University of Science and Technology, Nanjing 210094, People's Republic of China
[c] Institute of Modern Acoustics, Nanjing University, Nanjing 210093, People's Republic of China

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Abstract

The transient temperature fields generated by a pulsed laser in film-substrate system are obtained by using the finite element method. Time integrations of the semi-discrete finite element equations are achieved by using approximate one order derivative of temperature. The temperature dependences of material properties are taken into account, which has a great influence on the temperature fields indicated by the numerical results. The pulsed laser-induced transient temperature fields in aluminum/methyl-methacrylate system and aluminum/copper system are obtained, which will be useful in the research on thermoelastic excitation of laser ultrasonic waves in film-substrate system.

1. Introduction

During the process of laser–material interaction, due to the absorption of laser energy, transient temperature distribution will be generated in materials, which further produces the localized-zone strains in materials. This is the thermoelastic mechanism of pulsed laser-induced ultrasonic waves and a large amount of work has been devoted to solving the thermoelastic wave problems [1–4]. Rose [1] considered the laser as a surface heating source and neglected the thermal diffusion in SCOE model; McDonald [2] studied the effect of the thermal diffusion on the thermoelastic wave; Wang and Xu [4] took into account the non-Fourier effect in heat conduction in the case of the ultrafast laser-induced ultrasonics. However, Most of the previous papers neglected the temperature dependence and the thermal properties of the material and the absorptance of laser into the material. Actually, the temperature dependence of material parameters has an important influence on transient temperature distribution [5] and the resulted ultrasound waves. In order to develop the laser ultrasonic technique into an effective method of quantitative inspection, it is necessary to study the pulsed laser-induced transient temperature distribution and then establish the relation between the parameters of laser and the laser-induced ultrasonic waves.

Laser-induced surface acoustic wave in layered structure, especially film-substrate system, arise much interest in recent years [6,7] due to its potential in non-destructive evaluation of the parameters of films, coating and bonds on a substrate. So it is very important and necessary to analyze the transient temperature field in the film-substrate system. In this paper, we take into account the temperature-dependent thermal properties and use the finite element method (FEM) to analyze the transient temperature field in the film-substrate system.

* Corresponding author.
E-mail address: nxw@mail.njust.edu.cn (Z.H. Shen).

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Nomenclature

a_0	laser pulse spot radius
$A(T)$	absorptivity
C	heat capacity at constant pressure
$[C]$	heat capacity matrix
d	the thickness of the substrate
h	film thickness
k	thermal conductivity
$[K]$	conductivity matrix
N	shape function
$\{p_1\}$	heat flux vector
$\{p_2\}$	heat source vector
R	radius of the specimen
t_0	laser pulse rise time
T	temperature

Greek symbols

ρ	density, $\mathrm{kg\,m^{-3}}$
Δt	time step

Subscripts

f	film
s	substrate

2. Theory and numerical method

2.1. Thermal conduction theory

The geometry of laser irradiation on a film-substrate system is schematically shown in Fig. 1. The spatial mode of the laser beam is assumed as Gauss distribution so that a cylindrical coordinate system is adopted. The thermal conductive equation can be described as

$$\rho_i c_i \frac{\partial T_i(r,z,t)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rk_i \frac{\partial T(r,z,t)}{\partial r}\right) + \frac{\partial}{\partial z}\left(k_i \frac{\partial T_i(r,z,t)}{\partial z}\right) \tag{1}$$

where $T_i(r,z,t)$ represents the temperature distribution at time t, ρ_i, c_i, and k_i, are the density, thermal capacity and thermal conductive coefficient; $i = f, s$ represents the parameters in film-substrate respectively.

The laser irradiation is considered to serve as a surface heat source and temperature of the back surface of the system is supposed to be thermal insulation, so that the boundary conditions at these two surfaces can be written as

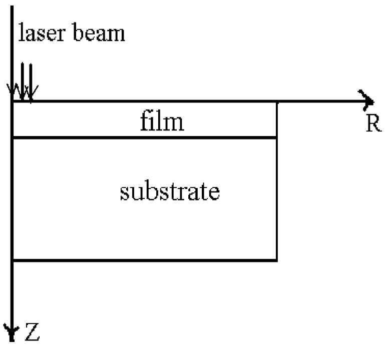

Fig. 1. Schematic diagram for laser irradiation film-substrate system.

$$-k_\mathrm{f} \frac{\partial T_\mathrm{f}(r,z,t)}{\partial z}\bigg|_{z=0} = I_0 A(T) f(r) g(t) \tag{2}$$

and

$$T_\mathrm{s}(r,z,t)|_{z=h+d} = T_0 \tag{3}$$

where I_0 is the incident laser power density, $A(T)$ is the optical absorptivity of the film, and T_0 is the ambient temperature and it is taken as 300 K. h and d are the thickness of the film and substrate respectively. $f(r)$ and $g(t)$ are the spatial and temporal distribution of the laser pulse. These two functions can be written as

$$f(r) = \exp\left(-\frac{r^2}{a_0^2}\right) \tag{4}$$

$$g(t) = \frac{t}{t_0}\exp\left(-\frac{t}{t_0}\right) \tag{5}$$

where a_0 is the radius of the pulsed laser spot, t_0 is the rise time of the laser pulse.

Thermal insulation is applied at the radial direction, so that

$$k\frac{\partial T}{\partial n}\bigg|_{r=0} = 0 \quad k\frac{\partial T}{\partial n}\bigg|_{r=R} = 0 \tag{6}$$

where R is the radius of the specimen.

Suppose a perfect thermal contact at the interface, we have

$$T_\mathrm{f}(r,z,t)|_{z=h} = T_\mathrm{s}(r,z,t)|_{z=h} \tag{7}$$

and

$$-k_\mathrm{f}\frac{\partial T_\mathrm{f}(r,z,t)}{\partial z}\bigg|_{z=h} = -k_\mathrm{s}\frac{\partial T_\mathrm{s}(r,z,t)}{\partial z}\bigg|_{z=h} \tag{8}$$

The initial condition is

$$T_i(r,z,0) = 0 \tag{9}$$

2.2. Finite element method

In order to investigate the temperature distribution induced by the laser irradiation in film-substrate system, the FEM [8,9] is adopted due to its flexibility in modeling layered structures and its capability in obtaining full field numerical solution. The heat-affected zone is much smaller than the domain of the material and the thickness of the film is in the range of μm, therefore, very fine meshes is demanded to resolve temperature distribution in the film and the irradiated region. Variable fine meshes shown in Fig. 2, close to the boundary of the heat flux and expanded gradually away from it, are used to obtain good accuracy with reasonable calculation time.

With the initial and boundary conditions, the weak formulation of heat conduction equation that describes the transient temperature distribution is obtained from the discrete domain. Discretizing the plane with axis symmetry into the nonoverlapping finite elements, we can get the associated matrix. Nodal points, defined as the shape functions N, are associated with this discretization. The solution of the Galerkin counterpart of the weak formulation is then expressed in terms of the shape functions and gives rise to the following finite element form of the heat conduction equation

$$[C]\{\dot{T}\} + [K]\{T\} = \{p\} \tag{10}$$

with the heat capacity matrix $[C] = \int\int_{S^e} \rho c N_i N_j \times (2\pi r)\,\mathrm{d}r\,\mathrm{d}z$, the conductivity matrix

$$[K] = \int\int_{S^e} \left[rK_r \frac{\partial N_i}{\partial r}\frac{\partial N_j}{\partial r} + rK_z \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z} \right] (2\pi r)\,\mathrm{d}r\,\mathrm{d}z$$

$\{p\} = \{p_1\} + \{p_2\}$, the heat flux vector

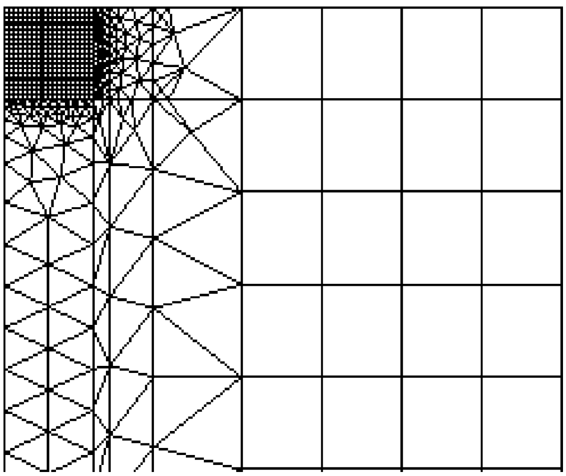

Fig. 2. Finite element meshes of the film-substrate system.

$$\{p_1\} = \int\int_{S^e} \dot{q} N_i 2\pi r\,\mathrm{d}r\,\mathrm{d}z$$

and the heat source vector

$$\{p_2\} = \int\int_{S^e} q N_i 2\pi r\,\mathrm{d}r\,\mathrm{d}z$$

where $\{T\}$ is the temperature vector, $\{\dot{T}\}$ is the temperature rate vector. T can be written as:

$$T(r,z,t) = \sum_{j=1}^{N} N_j(r,z) T_j(t) \tag{11}$$

In order to solve Eq. (10), time integration is performed. For the integration time step Δt, temperature and its first derivative can be approximately written as

$$T|_t = \frac{1}{2}(T_{i+1} + T_i) \quad \text{and} \quad \left.\frac{\mathrm{d}T}{\mathrm{d}t}\right|_t = \frac{T_{i+1} - T_i}{\Delta t} \tag{12}$$

where $T_{i+1} = T(t + \Delta t)$, $T_i = T(t)$. Substituting Eqs. (11) and (12) into Eq. (10), we obtain the following system of algebraic equations

$$\left(\frac{2[C]}{\Delta t} + [K]\right) T_{t+\Delta t} = \left(\frac{2[C]}{\Delta t} - [K]\right) T_t + (p) \tag{13}$$

Thus, Eq. (13) constitutes an algebraic problem at each time step. The most useful and versatile implementation is to form an "effective static problem". At each time step, the new temperatures are calculated. By continuous integrating Eq. (13) over $n\Delta t$ (where $n = 0, 1, \ldots,$ total number of time step), the entire time history of temperature is generated.

3. Numerical simulations and results

3.1. Laser and material parameters

Based on the theories described above, we have calculated the temperature fields in the film-substrate system. We suppose the thickness of the film and substrate are 10 μm and 1 cm respectively and the radius of the sample is 4 cm. The laser energy is 0.35 mJ, the pulse rise time t_0 and the radius of the pulsed laser spot on the sample surface are taken to be 10 ns and 50 μm, respectively. To compare the temperature fields of film on different substrates, we calculate two cases: aluminum film on methyl-methacrylate and on copper substrate.

The temperature dependence of absorptivity can be written as [10]

$$A_{\mathrm{Al}}(T) = 5.2 \times 10^{-2} + 3 \times 10^{-5}(T - 300) \tag{14}$$

where T is the temperature measured in Kelvin. The temperature dependence of thermal conductivities of aluminum, methyl-methacrylate and copper [11,12] can be expressed as

$$k_{\mathrm{Al}}(T) = \begin{cases} 292.6 & T < 200 \\ 249.45 - 0.085T & 200 < T < 730 \\ 198.47 - 0.014T & 730 < T_{\mathrm{m}} \end{cases} \tag{15}$$

$$k_{\text{methyl-methacrylate}}(T) = \begin{cases} 1.83 \times 10^{-5}T + 0.012 & 293 < T < 800 \\ 1.2 \times 10^{-5}T + 0.021 & 800 < T < T_{\mathrm{m}} \end{cases} \tag{16}$$

$$k_{\mathrm{Cu}}(T) = 410.83 - 0.045T \quad 293 < T < T_{\mathrm{m}} \tag{17}$$

where $k(T)$ is measured in $\mathrm{W\,m^{-1}\,K^{-1}}$.

The specific heat capacities of methyl-methacrylate are taken as 840 $\mathrm{J\,kg^{-1}\,K^{-1}}$, and the temperature dependence of aluminum and copper are

$$C_{\mathrm{Al}} = \begin{cases} 3.971T & T < 200 \\ 780.27 + 0.488T & 200 \leqslant T < T_{\mathrm{m}} \end{cases} \tag{18}$$

$$C_{\mathrm{Cu}}(T) = 0.13T + 345.38 \quad 200 \leqslant T < T_{\mathrm{m}} \tag{19}$$

where $C(T)$ is measured in $\mathrm{J\,kg^{-1}\,K^{-1}}$.

The densities of methyl-methacrylate is 2400 $\mathrm{kg\,m^{-3}}$ and the temperature dependence of density of aluminum and copper can be expressed as

$$\rho_{\mathrm{Al}} = -0.22T + 2769 \quad 300 \leqslant T < T_{\mathrm{m}} \tag{20}$$

$$\rho_{\mathrm{Cu}} = -0.49T + 9079 \quad 300 \leqslant T < T_{\mathrm{m}} \tag{21}$$

where ρ is measured in $\mathrm{kg\,m^{-3}}$, T_{m} is the melting point.

3.2. Numerical results

Fig. 3(a) shows the temperature evolution of the aluminum/methyl-methacrylate system at the center of laser irradiation in different depths. The surface temperature rises rapidly during the laser irradiation while the cooling process is relatively slow due to the thermal conductivity. With the increment of the depth, the velocity of the rising temperature decreases. Such a trend of temperature evolution is the same as that observed in aluminum/copper system, shown in Fig. 3(b).

The surface temperature evolutions at the center of laser irradiation in aluminum/copper system, both considering and neglecting the temperature dependences of material parameters are illustrated in Fig. 4, which indicates the influence of the temperature dependence of material properties on the transient temperature field. By neglecting the temperature dependence of material parameters and taking into account the temperature dependence of thermal conductivity, thermal capacity and density, the comparison curves of the numerical results are shown in Fig. 4(a). It can be seen from the figure that there is nearly no difference in the temperature rise and decrease stage, except for a little difference of the peak temperature. However, by taking the temperature dependence of absorptivity into consideration, the temperature rises more rapidly and decreases more slowly, which is shown in Fig. 4(b). In this case, the peak temperature is up to about 781 K, which is much higher than 704 K in the case of neglecting the temperature dependence of absorptivity. The numerical result considering the temperature dependence of all material parameters is shown in Fig. 4(c). Among all material parameters, we find that the temperature-dependence absorptivity is the key reason for this temperature variety through our calculation. Therefore, in order to effectively analyze laser-generated ultrasonic waves by thermoelastic mechanism, in accuracy analysis of temperature field induced by laser pulse, we should take into account the temperature dependence of material properties, especially the temperature dependence of absorptance.

Figs. 5 and 6 are the temperature distribution of the aluminum/methyl-methacrylate system and aluminum/copper system in depth direction (a) and in radial direction (b) at different time. It can be seen from these figures that the radial temperature distribution is smooth in both systems due to the smooth spatial distribution of the laser beam. However, there is an obvious discontinuation in temperature gradient at the

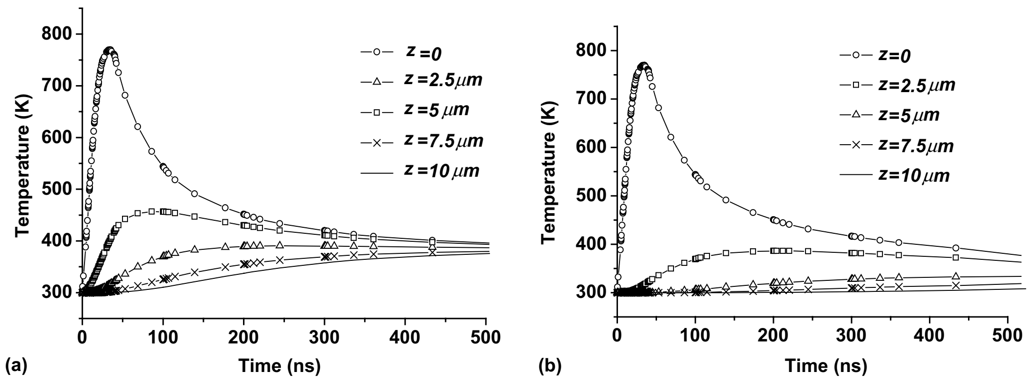

Fig. 3. The temperature evolution in different depths: (a) aluminum/methyl-methacrylate system ($r = 0$), (b) aluminum/copper system ($r = 0$).

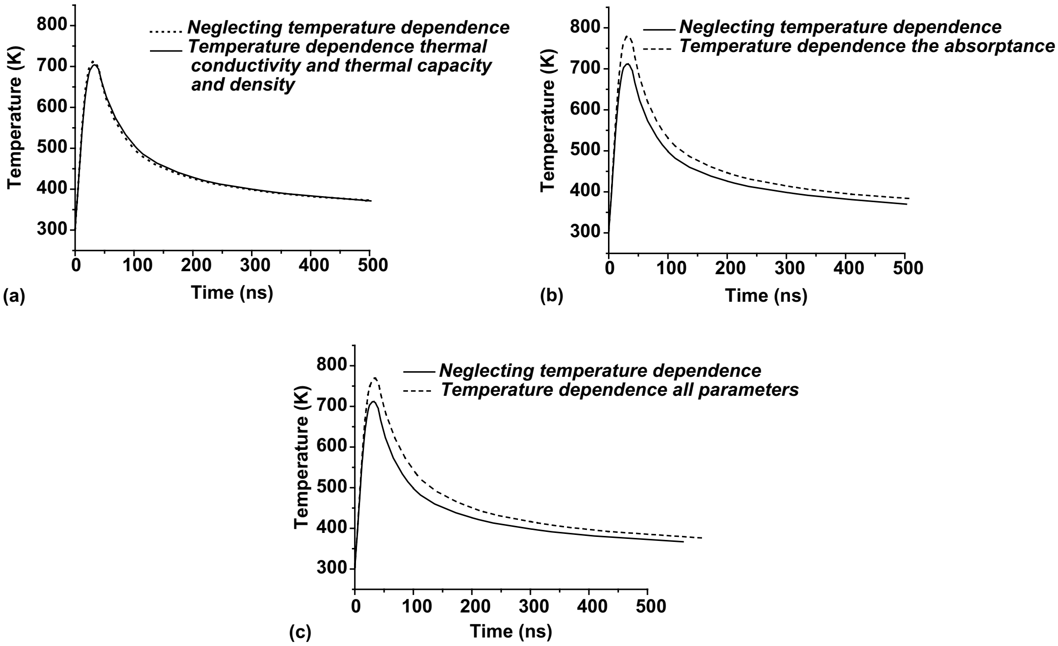

Fig. 4. The surface temperature evolution in aluminum/copper system considering and neglecting temperature dependence of material parameters ($z = 0$).

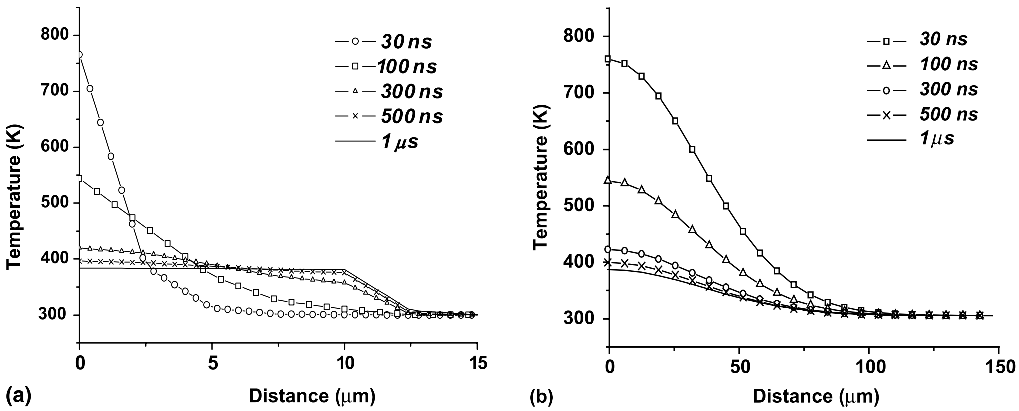

Fig. 5. Temperature distribution at various times in Al/methyl-methacrylate system: (a) depth direction, (b) radial direction.

interface between aluminum film and methyl-methacrylate substrate and the temperature variation in the substrate is much smaller than that in the film, which is due to the fact that the thermal conductivity of the methyl-methacrylate is much smaller than that of aluminum. There is a nearly smooth temperature transition in the aluminum/copper system, which is resulted from their thermal conductivities having the same order. The numerical results indicate that the temperature field in the substrate can be neglected for simplification in the researches on thermoelastic generation of laser ultrasonic waves if the thermal conductivity is much larger than that of the substrate.

4. Conclusion

The FEM is applied to the thermal analysis of layered structure, like film-substrate system, and the numerical results proved that the procedure is effective and versatile. The temperature dependences of material parameters are taken into account in the calculation, which has a great influence on the transient temperature fields and the temperature dependence of absorptivity is the key factor for the temperature variation. Therefore, the temperature dependence of laser absorptivity should be taken into consideration in any researches on thermoelastic generation of laser ultrasonic waves and related thermal

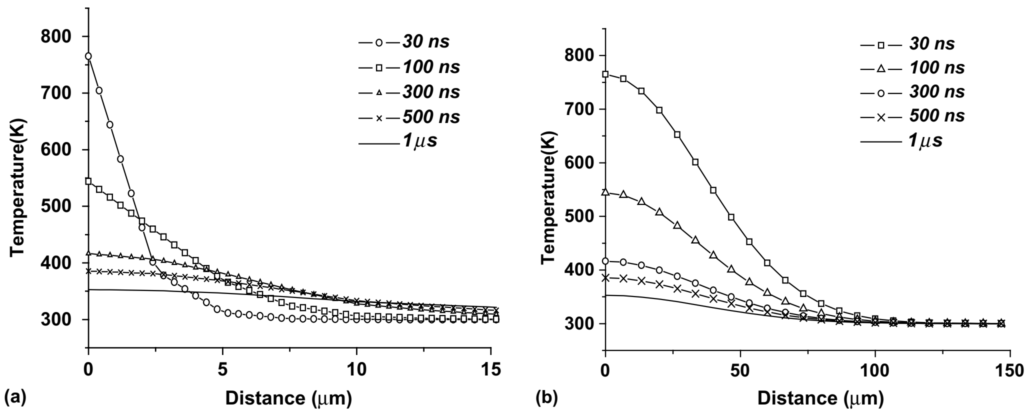

Fig. 6. Temperature distribution at various times in Al/copper system: (a) depth direction, (b) radial direction.

analysis. There is an obvious discontinuation in temperature gradient at the interface between aluminum film and methyl-methacrylate substrate and the temperature variation in the substrate is much smaller than that in the film, which is due to the fact that the thermal conductivity of the methyl-methacrylate is much smaller than that of aluminum. The numerical results indicate that the temperature field in the substrate can be neglected for simplification in the researches on thermoelastic generation of laser ultrasonic waves if the thermal conductivity is much greater than that of the substrate.

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References

[1] L.R.F. Rose, Point-source representation for laser-generated ultrasound, J. Acoust. Soc. Am. 75 (1984) 723–732.

[2] A.F. McDonald, On the precursor in laser-generated ultrasound waveforms in metals, Appl. Phys. Lett. 56 (1990) 230–232.

[3] R.J. Bemstein, J.B. Spicer, Line source representation for laser-generated ultrasound in aluminum, J. Acoust. Soc. Am. 107 (2000) 1352–1357.

[4] X. Wang, X. Xu, Thermoelastic induced by pulsed laser heating, Appl. Phys. A 23 (2001) 107–114.

[5] Z.H. Shen, S.Y. Zhang, Laser heating of a thin plate with time-dependent absorptance, Microwave Opt. Technol. Lett. 28 (2001) 364–367.

[6] T.W. Murry, S. Krishnaswamy, J.D. Achenbach, Laser induced ultrasonic waves in films and coatings, Appl. Phys. Lett. 74 (1999) 3561–3564.

[7] Z.H. Shen, S.Y. Zhang, Laser-induced ultrasonic waves in the film-substrate system, Prog. Nat. Sci. 11 (2001) s299.

[8] J.N. Reddy, An Introduction to the Finite Element Method, second ed., McGraw-Hill, New York, 1993.

[9] R.D. Cook, D.S. Malkus, M.E. Plesha, Concepts and Applications of Finite Element Analysis, third ed., John Wiley, New York, 1989.

[10] W.M. Rohsenow, J.P. Hartnett, E.N. Ganic, Handbook of Heat Transfer Fundamentals, second ed., McGraw-Hill, New York, 1985.

[11] F. Keith, S.B. Mark, Principles of Heat Transfer, fourth ed., Harper and Row, New York, 1986.

[12] S.K. Lee, W.S. Chang, S.J. Na, Numerical and experimental study on the thermal damage of thin Cr films induced by excimer laser irradiation, J. Appl. Phys. 86 (1999) 4282–4289.