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Finite element analysis of three-dimensional laser-induced transient thermal grating in diamond/ZnSe system*

Cheng Ying(程 营), Huang Qiao-Jian(黄巧建), and Liu Xiao-Jun(刘晓峻)†

Key Laboratory of Modern Acoustics of Ministry of Education, Nanjing University, Nanjing 210093, *China*

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This paper uses finite element method to obtain the three-dimensional temperature field of laser-induced transient thermal grating (TTG) for two-layered structure of diamond film on ZnSe substrate. The numerical results indicate that unique two-times heating process is gradually experienced in the area between two adjacent grating stripes. However, there is a little change for the temperature field along the depth direction for the diamond film due to its great thermal conductivity. It further finds that the thickness of the diamond film has a significant influence on the temperature field in diamond/ZnSe system. The results are useful for the application of laser-induced TTG technique in film/substrate system.

Keywords: thermal analysis, transient thermal grating, diamond/ZnSe, finite element method
PACC: 6500, 6610C, 7820B

1. Introduction

In recent years, the development of infrared (IR) materials in particular for the 8–12 μm spectral range has increased interest in the study of ZnSe.[1−5] ZnSe has a good transmittance property in the IR region, and hence a potential application in IR windows, especially for high-power IR lasers such as CO_2 laser at 10.6 μm and airborne IR sensor systems operating within the 8–12 μm atmospheric window. However, the mechanical, thermal and chemical properties of ZnSe are not enough to withstand severe environmental conditions such as abrasion, chemical attack or aerodynamic load. In order to improve the limits of ZnSe, one possible way is to use a diamond thin film as the protective coating on ZnSe due to the excellent mechanical and thermal properties.[1] In this case, the absorbed heat in diamond film due to photo-irradiation is considered to affect the properties of ZnSe window because of the worse transmission (0.03–0.05 cm^{-1} at 10.6 μm) of diamond film by a two orders of magnitude lower than that (0.0005 cm^{-1}) of ZnSe. Thus, the thermal analysis becomes very important to design the diamond/ZnSe system.

Many thermal analysis methods such as the laser-induced thermal analysis have been established in order to manufacture high-quality protective coating on ZnSe. For example, Yang *et al* analysed YbF_3/ZnSe system numerically using alternating direction-implicit technique.[6] However, most of them are difficult to be applied in diamond/ZnSe system because of the high thermal conductivity and small thickness for diamond film.[7] Recently, laser-induced transient thermal grating (TTG) technique is found to be an efficient way to determine the thermal diffusivities of bulk materials due to its advantages of non-contact and non-destruction.[8−11] However, no complete principle of the TTG technique is established for diamond/substrate system.[9,10] In order to develop the laser-induced TTG technique into an effective method of quantitative inspection for diamond/substrate system, it is necessary to study the transient temperature distribution generated by laser-induced TTG and then establish the relation between the parameters of materials and the temperature field. Therefore, it is meaningful to make theoretical analysis on thermal properties of diamond film heated by laser-induced TTG. The analysis of the temperature field for diamond/ZnSe system is significant and helpful for the measurement of the laser-induced TTG technique and the design of the diamond/ZnSe system.

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†Corresponding author. E-mail: liuxiaojun@nju.edu.cn

In this paper, finite element method (FEM) is introduced to simulate the temperature field of the two-layered diamond/ZnSe system by laser-generated TTG. The overall temperature distribution and the temperature evolution of the diamond/ZnSe system are presented. In order to investigate the influence of the thickness for the diamond film and the substrate effect on the temperature field, a thickness dependence of the diamond film is discussed in detail. We find that the temperature field in the diamond/ZnSe system is sensitive to the thickness of the diamond film.

2. Theory and numerical method

Before analysing the temperature field for diamond/ZnSe system, let us describe details of the TTG technique for determination of the thermal diffusivity in a two-layered film. As shown in Fig.1, two pulsed, intersecting, coherent pump beams (A and B) irradiate with a finite angle φ of inclination on the sample surface to produce interference bands of low and high irradiance. The excess heat due to the optical absorption within the sample generates a corresponding grating pattern of thermal expansion on the sample surface. This surface grating decays with time, since the associated spatially modulated, sinusoidal temperature field tends to equilibrate through thermal diffusion within the sample. The TTG signal is detected by measuring the diffracted intensity of a continuous-wave probe beam (indicated by C in Fig.1), and the thermal diffusivity of the sample can be extracted from the decay of the laser-probed TTG signal.[10] Here, L and Λ are thickness of the film and distance between the neighbouring stripes, respectively, which are described as well as the other symbols and subscripts used in this paper in Table 1. According Ref.[8], the distribution of the light intensity I in the sample can be expressed as

$$I = 2I_0(1-R)\exp(-\beta z)[1+\cos(2\pi x/\Lambda)]. \quad (1)$$

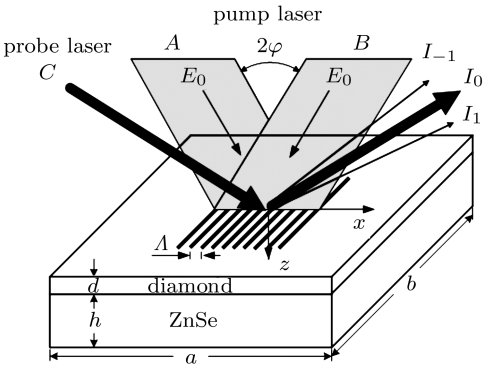


Fig.1. Optical configuration of TTG technique on a two-layered film. A and B are two pulsed, intersecting, coherent pump beams irradiate with a finite angle 2φ of inclination on sample. C is the continuous probe beam. L is thickness of the film. Λ is distance between the neighbouring stripes.

Table 1. Nomenclature of symbols and subscripts in this paper.

a, b/m	length and width of the sample	$[\boldsymbol{N}]$	interpolation function array
$c/(\mathrm{J\cdot kg^{-1}\cdot K^{-1}})$	specific heat	$[\boldsymbol{P}]$	temperature-load array
d/m	film thickness	$[\boldsymbol{\Phi}]$	temperature array
h/m	thickness of the substrate		
m	number of layers	Greek symbols	
r_0/m	laser radius	$\alpha/(\mathrm{m^2\cdot s^{-1}})$	thermal diffusivity
t_0/s	rise time of laser pulse	$\beta/\mathrm{m^{-1}}$	optical absorption coefficient
t/s	time	$\kappa/(\mathrm{W\cdot m^{-1}\cdot K^{-1}})$	heat conductivity
x, y, z	cylindrical coordinate	$\rho/(\mathrm{kg\cdot m^{-3}})$	density
I_0	intensity of pump laser	Λ	thermal grating constant
Q_0	absorbed laser energy of a pulse		
R	reflection index	subscripts	
T/K	temperature	i	material layer
$[C]$	heat-capacity matrix	V	element volume
$[K]$	heat-conduction matrix	e	element

The excess heat due to the optical absorption within the sample generates a corresponding grating pattern due to thermal expansion on the sample surface. If the illuminating pulsed laser is a Gaussian beam with radius r_0, the absorbed optical energy is then transformed as a heat source in m-layered media, which can be written as[12]

$$Q(x,y,z,t)=\frac{Q_0}{\pi r_0^2}(1-R)[1+\cos(2\pi x/\Lambda)]\prod_{i=1}^{m}\beta_i\exp\left(-\frac{x^2+y^2}{r_0^2}\right)\exp\left[-\left(\sum_{i=1}^{m-1}(\beta_i)-\beta_m\right)d_i+\beta_m z\right]g(t), \quad (2)$$

where $g(t)=\dfrac{t}{t_0^2}\exp\left(-\dfrac{t}{t_0}\right)$ represents the laser pulse shape.

The temperature distribution $T(x,y,z,t)$ satisfies the thermal diffusion equation

$$\nabla^2 T_i(x,y,z,t)-\frac{1}{\alpha_i}\frac{\partial T_{\rm i}(x,y,z,t)}{\partial t}=-\frac{Q(x,y,z,t)}{\kappa_i}, \quad (3)$$

where $T_i(x,y,z,t)$ represents the temperature distribution at time t, and i indicates the material layer. In the two-layered diamond/ZnSe structure, the laser irradiation (at 10.6 μm) is considered to act as a heat source in the diamond film, and the ZnSe substrate is regarded as transparent to the pulsed laser. The initial and boundary conditions can be written as

$$T(x,y,z,t)\,|_{t=0}=300, \quad (4)$$

$$\frac{\partial T(x,y,z,t)}{\partial x}\,|_{x=\pm\frac{a}{2}}=\frac{\partial T(x,y,z,t)}{\partial y}\,\Big|_{y=\pm\frac{b}{2}}=0, \quad (5)$$

$$\frac{\partial T(x,y,z,t)}{\partial z}\,|_{z=0}=\frac{\partial T(x,y,z,t)}{\partial z}\,|_{z=d+h}=0. \quad (6)$$

Supposing that there is a perfect thermal contact at the interface between the diamond film and the substrate, we have

$$T_{\rm f}(x,y,z,t)\,|_{z=d}=T_{\rm s}(x,y,z,t)\,|_{z=d} \quad (7)$$

and

$$-\kappa_{\rm f}\frac{\partial T_{\rm f}(x,y,z,t)}{\partial z}\,|_{z=d}=-\kappa_{\rm s}\frac{\partial T_{\rm s}(x,y,z,t)}{\partial z}\,|_{z=d}\ , \quad (8)$$

where the subscript f and s stands for the film and substrate, respectively.

In order to investigate the temperature distribution heated by laser-induced transient thermal grating in the film-substrate system, the FEM is adopted due to its flexibility in modelling layered structures and its preponderance to get full field numerical solution.[13,14] The general FEM form of heat conduction Eq.(3) can be written by

$$[\boldsymbol{C}]\{\dot{\boldsymbol{\Phi}}\}+[\boldsymbol{K}]\{\boldsymbol{\Phi}\}=\{\boldsymbol{P}\}, \quad (9)$$

where the elements of heat capacity matrix $[\boldsymbol{C}]$, heat conduction matrix $[\boldsymbol{K}]$ and temperature-load array $\{\boldsymbol{P}\}$ can be expressed by

$$\begin{aligned}C_{ij}&=\sum_e\int_{V_e}\rho c N_i N_j {\rm d}V,\\ K_{ij}&=\sum_e\int_{V_e}\left[k_x\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}+k_y\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}\right.\\ &\quad\left.+k_z\frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z}\right]{\rm d}V \end{aligned} \quad (10)$$

and

$$P_i=\sum_e\int_{V_e}qN_i{\rm d}V. \quad (11)$$

Therefore, combining the initial and boundary conditions of Eqs.(4)–(8), we can obtain the temperature field by solving Eqs.(9)–(12) with central difference method.

3. Numerical results and discussion

Based on the theory described above, we have calculated the temperature field in the diamond/ZnSe system. In our calculations, we suppose that the thickness d of the diamond film changes from 5 μm to 50 μm, while that of the substrate is maintained to be 0.2 mm. Because the d-value is in the range of μm, very fine meshes are required to resolve temperature distribution in the film. Therefore, we compress the model without affecting the overall thermal analysis and assume that both the length a and the width b of the samples equal to 1.7 mm. Moreover, the optical and thermal parameters of the diamond and the substrate are listed in Table 2.[15,16] In addition, the rise time t_0 and the radius r_0 of the pulsed laser are taken to be 3 ns and 1 mm, respectively. The absorbed laser energy Q_0 is deemed to be 20 J and the thermal grating constant Λ is 100 μm.

The top-viewed contour graphs of transient temperature field of the diamond/ZnSe system with $d=10\,\mu$m at various times t are shown in Fig.2, where (a), (b), (c) and (d) correspond to the time t of 1.5, 9, 54, 400 ns, respectively. The heating process and heat diffusion of the thermal grating induced by the pulsed

Table 2. Optical and thermal parameters of diamond and ZnSe.

	density/$(\mathrm{Kg}\cdot\mathrm{m}^{-3})$	specific heat/ $(\mathrm{J}\cdot\mathrm{kg}^{-1}\cdot\mathrm{K}^{-1})$	thermal conductivity/$(\mathrm{W}\cdot\mathrm{m}^{-1}\cdot\mathrm{K}^{-1})$	absorption coefficient at infrared light range/m^{-1}
diamond film	3500	509	2300	5
ZnSe	5360	335	19	~ 0

laser are clearly observed. During the short period (0–9 ns), the thermal grating is formed and the temperature increases abruptly due to the absorption of laser energy in the diamond film, as shown in Figs.2(a) and 2(b). In the following subsequence, the temperature of the diamond film decreases quickly as a result of the high thermal conductivity for the diamond. Moreover, the thermal grating becomes smeared with the passage of the time, as shown in Figs.2(c) and 2(d). The heat propagates from the film to substrate with the time processing.

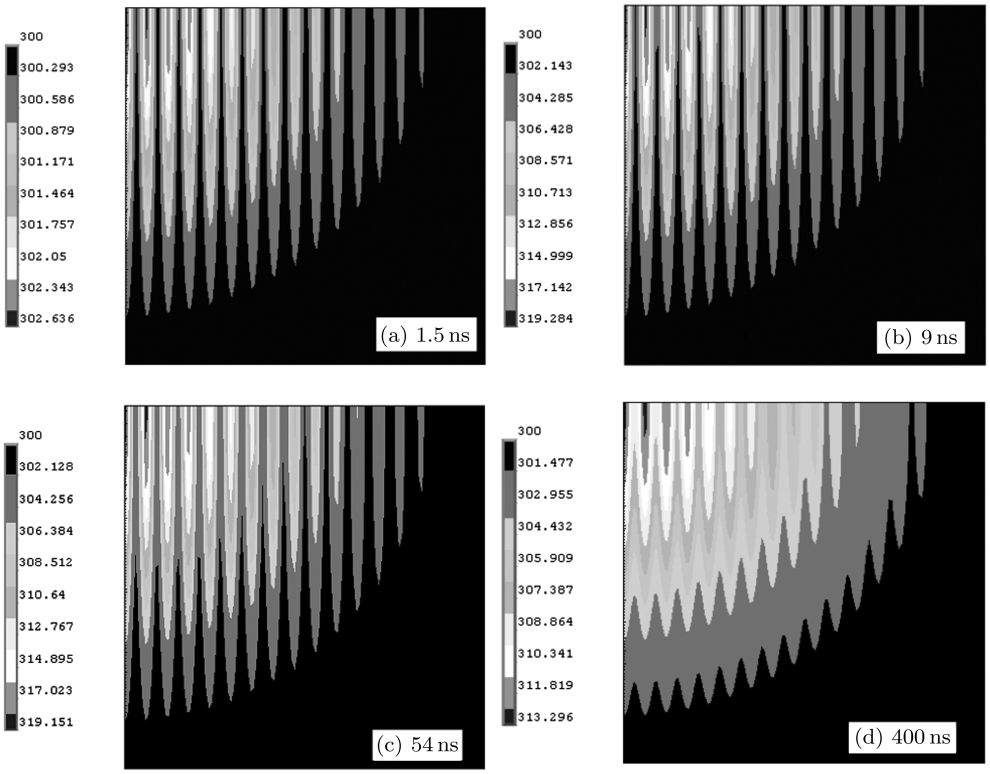


Fig.2. Top-viewed contour graphs of the transient temperature field for diamond/ZnSe system at different times: (a)–(d) correspond to the time of 1.5, 9, 54, 400 ns, respectively.

We further investigate the temperature evolution in the diamond/ZnSe system at the centre of laser irradiation $(x, y = 0)$ in different depths z. In Fig.3, the solid, dash, dot and dash-dot curves represent the calculated results for $z = 0$, 2.8, 6.1 and 10 μm, respectively. We find that the surface temperature at $z = 0\,\mu$m rises rapidly during the pulsed laser irradiation ($\sim$9 ns), and then decreases due to the thermal diffusion in the film. With the increment of the depth z, the peak temperature and the rate of the temperature-rising decrease, which are ascribed to the less absorbed energy in the deeper location and the heat propagation process from the top to substrate.

Figure 4 shows the time dependence of the surface temperature along the grating direction (x direction) at various x-values: solid, dash, dot, dash-dot and dash-dot-dot curves correspond to $x = 0$, 12, 24, 35 and 47 μm, respectively. With increasing x-value, the peak value of the temperature decreases due to the Gaussian space distribution of the laser heating. When the x-value reaches 24 μm, which is just smaller than the quarter of the thermal grating constant

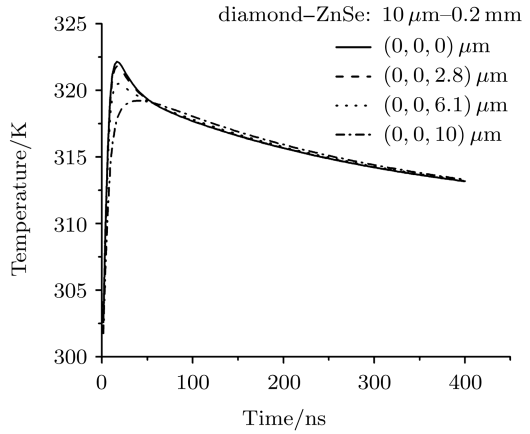


Fig.3. Temperature evolution of the diamond/ZnSe system at the centre of laser irradiation ($x = y = 0$) in different depths z: solid, dash, dot and dash-dot curves correspond to $z = 0$, 2.8, 6.1 and 10 μm, respectively.

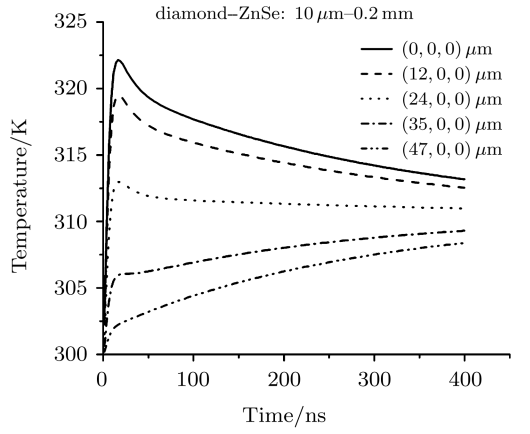


Fig.4. Time dependence of the surface temperature for diamond/ZnSe system along the grating direction (x direction): solid, dash, dot, dash-dot and dash-dot-dot curves correspond to $x = 0$, 12, 24, 35 and 47 μm, respectively.

($\Lambda/4 = 25\,\mu$m), the two times heating is experienced. The first time heating is generated by the direct heating with the laser pulse, whereas, the two times heating is induced by the thermal energy released from the thermal grating with higher temperature. With further increasing the x-value to 47 μm, which is close to the half of the thermal grating constant, the phenomenon for the two times heating becomes significant.

In order to find the film-thickness influence on the temperature field in the film/substrate system, we calculate the temperature fields with changing the thickness d of the diamond film in the range from 5 μm to 50 μm, while fixing the thickness of the substrate to be 0.2 mm. Figures 5(a) and 5(b) show the temperature evolution at two representative positions of (0, 0, 0) and (35 μm, 0, 0) with different thickness of the diamond films, respectively. The overall tendency of the temperature evolution does not change distinctly with increasing the d-value, as shown in Fig.5(a). We find that both the peak temperature and the decay rate increase, which are ascribed to the more absorbed laser energy for the thicker diamond film. As shown in Fig.5(b), the two times heating can also be clearly observed. One can easily observe that there exist significant inflection points at about 9 ns between two heating processes. The first part from 0 to 9 ns is direct heating due to the laser absorption, while the second part from 9 to 400 ns is indirect heating resulting from heat transferring. By comparing Fig.5(a) with Fig.5(b), we can clearly find the speed of the heat transferring from high temperature section in the

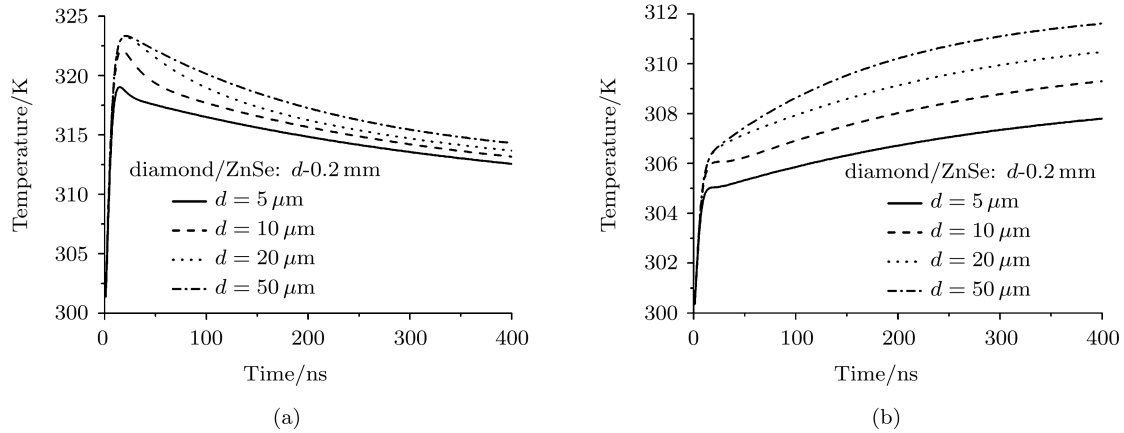


Fig.5. Temperature evolution for diamond/ZnSe system at (a) $x = 0$ and (b) $x = 35\,\mu$m with different thickness d of the diamond films: solid, dash, dot and dash-dot curves correspond to $d = 5$, 10, 20 and 50 μm, respectively.

middle of the stripe to the central points between two adjacent stripes. Due to the absorbed heat is easily transmitted to the deeper position (z-direction), the phenomenon of the two times heating becomes smooth with further increasing of the thickness of the diamond film.

With the obtained transient temperature field, we can further determine the displacements of the sample surface due to thermal expansion effect. Large deformation occurs in high temperature section while small displacement emerges in low temperature part. The surface grating decays with time, since the associated spatially modulated, sinusoidal temperature field tends to equilibrate through thermal diffusion within the sample. The time-variable TTG signal can be detected by measuring the diffracted intensity of a probe beam, as shown in Fig.1. Thus, the thermal diffusivity information of the diamond film can be extracted from the simulation of decay for the TTG signal.

4. Summary

We have calculated the three-dimensional temperature fields in the diamond/ZnSe system irradiated by laser-induced TTG with FEM. We find that the thickness of the diamond film has significant influence on the temperature distribution in the film. The peak temperature in the laser-irradiated centre abruptly increases, whereas the two times heating becomes obscure with increasing the thickness of the diamond film. Our results indicate that TTG technique may be a good method to characterize the thermal properties of the diamond/ZnSe system.

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