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Technical Note

Two-dimensional transient thermal analysis of diamond/Si structures heated by a pulsed circular Gaussian laser beam

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Abstract

Based on a 2D temperature model in cylindrical coordinate for multilayer thin films irradiated by a Gaussian laser beam, the 2D temperature field for two-layer structures of a transparent diamond thin film on an opaque silicon substrate is obtained by using FEM method. Besides, the influence of the heat conductivity of the diamond film on surface temperature of the bilayered structures is also calculated. The results show that it may be a good method by using the surface temperature attenuation curves to characterize the heat conductivity of the diamond film.

1. Introduction

Recently, diamond thin films are widely used in thermal managements of microelectronics, optics and sensors, due to its large heat conductivity [1]. However, the high thermal diffusivity, transparency and small thickness of diamond films make the thermal properties of the thin film even more difficult to be measured than for other materials [2]. Now many laboratories are trying to develop more acute and convenient methods to characterize the thermal properties of diamond thin films. On the other hand, pulsed laser techniques are widely used for characterizing the thermal properties of bulk materials. Therefore, it is meaningful to make theoretical analyses on the thermal properties of the diamond films deposited on substrates characterized by pulsed laser techniques.

The optical and thermal fields of multilayer thin films deposited on substrates irradiated by a pulsed laser beam have been studied theoretically by several authors [3–5]. However, most of the works were limited to one-dimensional (1D) problem. Besides, Nakano et al. [6] and Bianco and Manca [7] performed the two-dimensional (2D) thermal analysis of the multilayer thin films, such as a-Si, c-Si and TCO, etc., on glass substrates. In other words, the films with optical absorption deposited on transparent substrates were considered in the mentioned research work. However, the 2D thermal field for the multilayer structures concerned a transparent diamond film deposited on an opaque substrate Si wafer so far has not ever been carried out.

In this paper, based on a 2D model for multilayer thin films irradiated by a circular Gaussian laser beam, the thermal field distribution for a bilayered structure of a diamond film on a Si substrate is obtained by a numerical calculation of the finite element method (FEM). The influence of the heat conductivity variation of the diamond film on the surface temperature of the bilayered structures is also discussed. Therefore, the theoretical analyses combined with the related experiments can be used to characterize the thermal properties of the films.

2. Theory

When a pulsed laser beam is incident on the surface of a cylindrical sample with *m*-layered structure, the

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Nomenclature

c	specific heat, $\mathrm{J\,kg^{-1}\,K^{-1}}$
C	heat-capacity matrix
d	film thickness, m
g	laser pulse shape
K	heat-conduction matrix
L	thickness of the sample, m
m	number of layers
N	interpolation function array
P	temperature-load array
Q_0	absorbed laser energy of a pulse
R_0	radius of the sample, m
r, z	cylindrical coordinate
r_0	laser radius, m
t	time, s
t_0	rise time of laser pulse, s
T	temperature, K
Greek symbols	
α	thermal diffusivity, $\mathrm{m^2\,s^{-1}}$
β	optical absorption coefficient, $\mathrm{m^{-1}}$
κ	heat conductivity, $\mathrm{W\,m^{-1}\,K^{-1}}$
ρ	density, $\mathrm{kg\,m^{-3}}$
Φ	temperature array
Subscripts	
i	material layer
V	element volume
Superscripts	
T	transposed operator
e	element

absorbed optical energy is then transformed as a heat source in the media. If the illuminating pulsed laser is a Gaussian beam with radius r_0, based on the expression of heat power density for a single layer [8]

$$Q(r,z,t) = \frac{Q_0\beta}{2\pi r_0^2}\exp(-r^2/r_0^2)\exp(-\beta z)g(t), \tag{1}$$

the heat power density of the heating source for m-layered structures can be deduced as [6]

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

where $g(t)$ is laser pulse shape. For a Q-switched laser

$$g(t) = t\exp(-t/t_0)/t_0^2. \tag{3}$$

Then the thermal diffusion equation is

$$\nabla^2 T_i(r,z,t) - \frac{1}{\alpha_i}\frac{\partial T_i(r,z,t)}{\partial t} = -\frac{Q(r,z,t)}{\kappa_i}, \tag{4}$$

where $i = 1,2,\ldots,m$. In this work, the optical and thermophysical properties of the materials are considered independent of the temperature. The initial and boundary conditions are

$$T(r,z,t)|_{t=0} = 0, \tag{5}$$

$$T_i|_{z=d_i} = T_{i+1}|_{z=d_i}, \tag{6}$$

$$\kappa_i\frac{\partial T_i(r,z,t)}{\partial z}\bigg|_{z=d_i} = \kappa_{i+1}\frac{\partial T_{i+1}(r,z,t)}{\partial z}\bigg|_{z=d_i}, \tag{7}$$

$$\frac{\partial T(r,z,t)}{\partial z}\bigg|_{z=0} = \frac{\partial T(r,z,t)}{\partial z}\bigg|_{z=L} = 0, \tag{8}$$

$$\frac{\partial T(r,z,t)}{\partial r}\bigg|_{r=R_0} = 0. \tag{9}$$

Since the problem we are interested lasts only a few hundred nanoseconds, the heat convection and radiation are not considered here.

It is very difficult to solve Eq. (4) analytically. A numerical method of FEM is employed for solving the equation. The general FEM form can be written by

$$\begin{bmatrix} C_1 & 0 & \cdots & 0 \\ 0 & C_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & C_m \end{bmatrix}\begin{bmatrix} \dot{\Phi}_1 \\ \dot{\Phi}_2 \\ \vdots \\ \dot{\Phi}_m \end{bmatrix} + \begin{bmatrix} K_1 & 0 & \cdots & 0 \\ 0 & K_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & K_m \end{bmatrix}\begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_m \end{bmatrix} = \begin{bmatrix} P_1 \\ P_2 \\ \vdots \\ P_m \end{bmatrix}, \tag{10}$$

where $\dot{\Phi}_i = \mathrm{d}\Phi/\mathrm{d}t$. The C_i, K_i and P_i can be expressed by

$$K_i = \sum\int_{V^e}\kappa_i\left(\left(\frac{\partial N}{\partial r}\right)^{\mathrm{T}}\left(\frac{\partial N}{\partial r}\right) + \left(\frac{\partial N}{\partial z}\right)^{\mathrm{T}}\left(\frac{\partial N}{\partial z}\right) - \left(\frac{\partial N}{\partial z}\right)^{\mathrm{T}}\left(\frac{N}{r}\right)\right)\mathrm{d}V, \tag{11}$$

$$C_i = \sum\int_{V^e}\rho_i c_i N^{\mathrm{T}} N\,\mathrm{d}V, \tag{12}$$

Table 1
Physical parameters of diamond and silicon [9]

	Specific heat ($J\,kg^{-1}\,K^{-1}$)	Density ($kg\,m^{-3}$)	Heat conductivity ($W\,m^{-1}\,K^{-1}$)	Absorption coefficient (m^{-1})
Diamond	509	3500	2300	
Silicon	712	2330	148	1.0×10^6

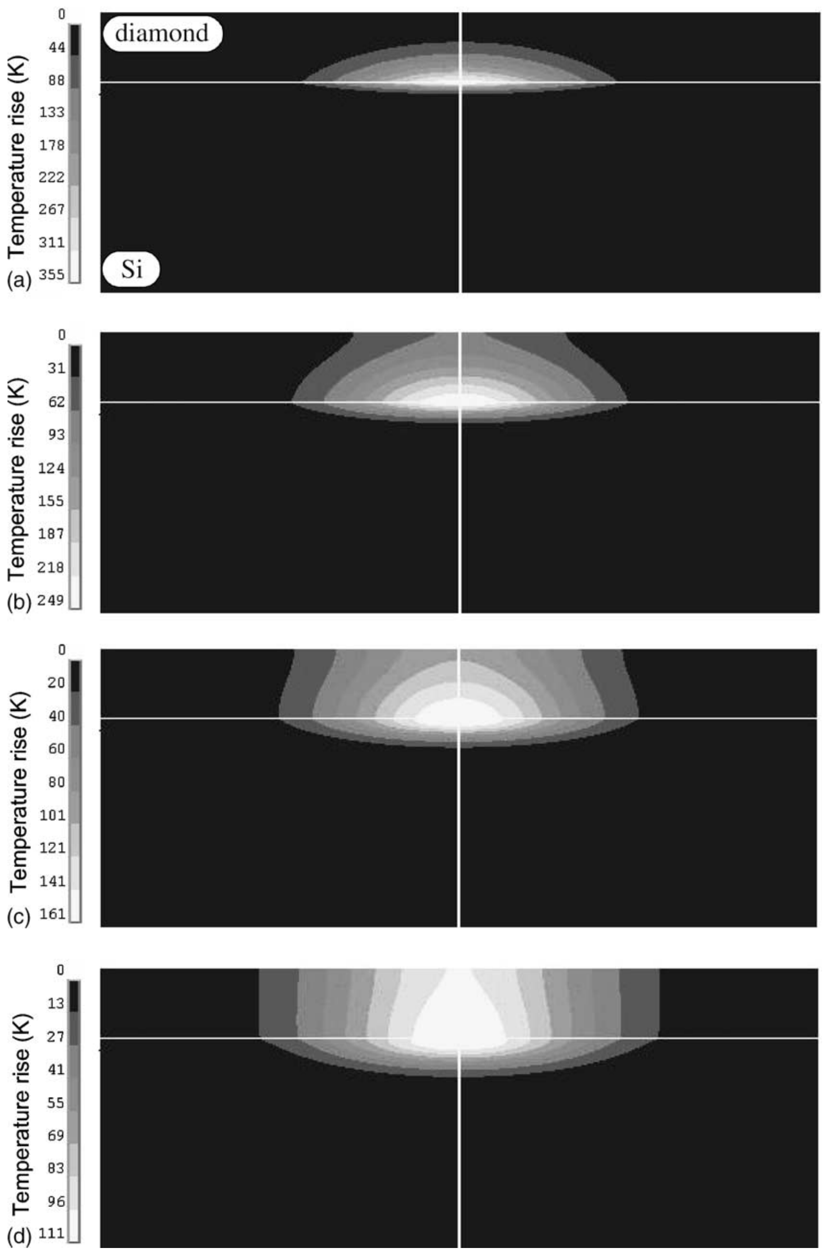

Fig. 1. Contour map of transient temperature field at different times (as $t_0 = 4.0$ ns and $r_0 = 15$ μm): (a) 8.4, (b) 18.4, (c) 28.4 and (d) 43.4 ns.

$$P_i = \sum \int_{V^e} \rho_i Q_i N^{\mathrm{T}} \, \mathrm{d}V. \tag{13}$$

Thus, combining the initial and boundary conditions of Eqs. (5)–(9), by solving Eqs. (10)–(13) with central difference method, the temperature field can be obtained.

3. Numerical results and discussion

For bilayered structures of a thin diamond film deposited on a silicon substrate, however, when a pulsed laser illuminates on the surface, the laser beam penetrates the diamond film with a little absorption and then is absorbed in a very thin layer beneath the diamond/silicon interface, because the absorption of diamond is weak whereas the absorption of silicon is strong [10].

Furthermore, the thicknesses of the diamond film and silicon substrate are taken to be 10 and 100 μm, respectively, and the sample radius is 50 μm. Meanwhile, the optical and thermal parameters for silicon and diamond are listed in Table 1. In addition, the pulse time t_0 and the laser radius r_0 are taken to be 4.0 ns and 15 μm, respectively. The absorbed laser energy Q_0 is taken 4.0×10^{-6} J and the initial temperature of the sample is assumed to be zero.

The contour map of transient temperature field calculated at different times is shown in Fig. 1, in which (a)–(d) correspond to the time of 8.4, 18.4, 28.4 and 43.4 ns, respectively. From the figure, we can clearly see the process of heat conduction and the temperature distribution at the near interface region of diamond and silicon. Heating first takes place in a very thin layer beneath the diamond/silicon interface, as shown in Fig. 1(a). Due to the high conductivity of the diamond, heat propagates much faster in the diamond film than in the silicon substrate. In Fig. 1(b), the heat propagates up to the surface of the diamond film and diffused in the film, whereas it propagates down only about 2 μm in the

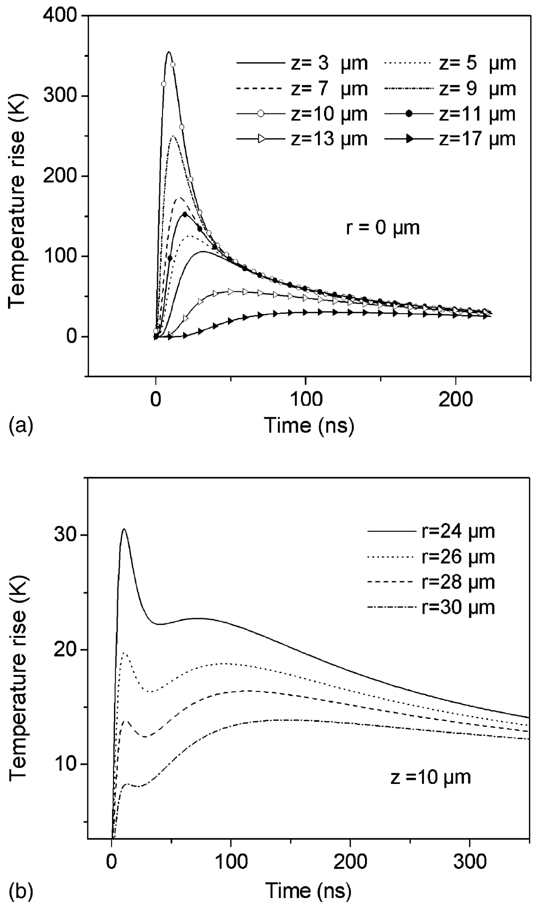

Fig. 2. Dependence of the temperature field on time (as $t_0 = 4.0$ ns and $r_0 = 15$ μm): (a) in different depths, 3–17 μm at $r = 0$, (b) in different r, 24–30 μm at the interface.

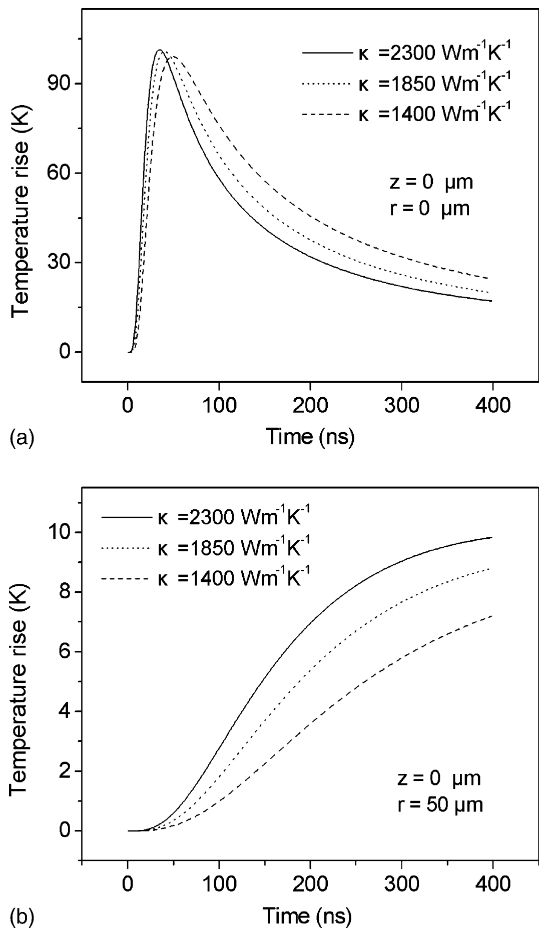

Fig. 3. Influence of heat conductivity of diamond film on surface temperature (as $t_0 = 4.0$ ns and $r_0 = 15$ μm): (a) $r = 0$, (b) $r = 50$ μm.

silicon substrate. The similar phenomenon can be observed in Fig. 1(c) and (d).

Fig. 2 shows the dependence of the temperature field on time in different depths or radii, where (a) is the temperature field in z-direction at $r = 0$ and (b) is in r-direction at the interface. From Fig. 2(a) we can see that, at the pulsed laser incident location, the temperature at the interface (10 μm in z-direction) rises drastically, which shows that the most energy is absorbed there. Then, with time increases, the temperature in the film decreases and the temperature in substrate increases gradually, which show that the absorbed large number of thermal energy in the film becomes the heating resource for the substrate. Fig. 2(b) shows the condition at the interface, where r lies between about 24 and 30 μm, two times heating are experienced. Obviously, the first heating is induced by the direct heating by the laser pulse, whereas, the second one is just induced by the thermal energy releases from the heated diamond film. Actually, the phenomenon of two times heating can be found in the region near the interface where r is greater than 20 μm.

Additionally, the influence of heat conductivity of diamond film on surface temperature is also calculated, as shown in Fig. 3. In Fig. 3(a), when heat conductivity of the diamond film changes from 1400 to 2300 $\mathrm{W\,m^{-1}\,K^{-1}}$, the variation of surface temperature with time in the rising part of the curve changes few, whereas the variation of surface temperature in the attenuating part changes with higher values. Therefore, the attenuating part of the temperature curve is more sensitive to the variation of the heat conductivity of diamond film than the rising part. Compared with Fig. 3(a) and (b), the influence of heat conductivity on surface temperature in the center of laser beam irradiation is greater than that in the other places.

4. Conclusion

A 2D temperature field model for multilayered thin films irradiated by a Gaussian laser beam is presented. Then, by using the FEM method, the 2D temperature field for a bilayered structures of a transparent diamond thin film on an opaque silicon substrate is obtained, where the diamond film can be considered as transparent and light absorption takes place in a very thin layer beneath the interface (including the interface) of the film and the substrate.

Due to the high heat conductivity of the diamond film, most of the heat energy diffuses fast to the diamond film in the region near the interface. Then, the region acts as a heat reservoir and diffuses the absorbed heat energy to the substrate after the laser pulse vanishes. As a result, the phenomenon of two times heating can be clearly observed in the region near the interface where r is greater than 20 μm.

Furthermore, the influence of the heat conductivity variation of the diamond film on surface temperature of the bilayered structures is also achieved. The result shows that it may be a good method by using the surface temperature attenuation curves to characterize the heat conductivity of the transparent diamond film.

Acknowledgements

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