Analysis of laser induced thermal mechanical relationship of HfO_2/SiO_2 high reflective optical thin film at 1064 nm

Gang Dai (戴　罡)*, **Yanbei Chen (陈彦北)**, **Jian Lu (陆　建)****, **Zhonghua Shen (沈中华)**, **and Xiaowu Ni (倪晓武)**

School of Science, Nanjing University of Science and Technology, Nanjing 210094, China

**E-mail: huma_1@163.com; **e-mail: lujian@mail.njust.edu.cn*

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A numerical model is developed for the calculation of transient temperature field of thin film coating induced by a long-pulsed high power laser beam. The electric field intensity distribution of HfO_2/SiO_2 high reflective (HR) film is investigated to calculate the thermal field of the film. The thermal-mechanical relationships are discussed to predict the laser damage area of optical thin film under long pulse high energy laser irradiation.

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The problem of laser damage in optical materials has been investigated for more than 40 years[1] because the damage of optical components often represents a limitation in laser performance. Coated components show a lower resistance than bulk materials, therefore, analysis is concentrated on thin film materials. Most attention is paid to the studies of short-pulse laser irradiation damage. As a result, damage mechanisms for short-pulse irradiation are now well understood[2−9]. However, there are little relevant reports on the millisecond long pulse laser induced damage in optical thin films. Therefore, it is significant to investigate the thermal-mechanical relationship of multilayer during long pulse laser irradiation.

A numerical model is established to study the thermal-mechanical relationship of optical thin films under long pulse laser irradiation. The electric field pattern of HfO_2/SiO_2 high reflective (HR) film at 1064-nm laser is calculated. Thermal field distribution is calculated according to the electric intensity, and the thermal-stress is computed as well.

The electromagnetic field of laser obeys the Maxwell Equation during the propagation in multilayer as follows:

$$\frac{\mathrm{d}}{\mathrm{d}z^2}+\left(\frac{2\pi n_k}{\lambda}\right)^2 E_k(\mathrm{z})=0, \tag{1}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}E_k(z)+\mathrm{i}\frac{2\pi n_k}{\lambda}H_k(\mathrm{z})=0, \tag{2}$$

where E_k,H_k are electric field and magnetic field in layer k, respectively, n_k is the refractive index of layer k, and λ is the wavelength of the light. We take the layer next to the substrate as layer one, and the top layer as layer N. The typical construction of HfO_2/SiO_2 HR film at 1064 nm is $\mathrm{G}\,|(\mathrm{HL})^{\wedge}\,12\mathrm{H}|\,\mathrm{A}$, as shown in Fig. 1, where, G indicates K9 glass, H and L represent a quarter-wave optical thickness of high (HfO_2) and low (SiO_2) refractive index materials, respectively, and A is air.

The characteristic matrix[10] of the film could be expressed as

$$\begin{bmatrix} B_j \\ C_j \end{bmatrix}=\begin{bmatrix} \cos\delta & \frac{\mathrm{i}}{n_1}\sin\delta \\ \mathrm{i}n_1\sin\delta & \cos\delta \end{bmatrix}\begin{bmatrix} 0 & \frac{\mathrm{i}}{n_2} \\ \mathrm{i}n_2 & 0 \end{bmatrix}\begin{bmatrix} 0 & \frac{\mathrm{i}}{n_1} \\ \mathrm{i}n_1 & 0 \end{bmatrix}\cdots\begin{bmatrix} 0 & \frac{\mathrm{i}}{n_2} \\ \mathrm{i}n_2 & 0 \end{bmatrix}\begin{bmatrix} 0 & \frac{\mathrm{i}}{n_1} \\ \mathrm{i}n_1 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ n_g \end{bmatrix}, \quad \frac{j+1}{2}=N, \tag{3}$$

$$\begin{bmatrix} B_j \\ C_j \end{bmatrix}=\begin{bmatrix} \cos\delta & \frac{\mathrm{i}}{n_2}\sin\delta \\ \mathrm{i}n_2\sin\delta & \cos\delta \end{bmatrix}\begin{bmatrix} 0 & \frac{\mathrm{i}}{n_1} \\ \mathrm{i}n_1 & 0 \end{bmatrix}\begin{bmatrix} 0 & \frac{\mathrm{i}}{n_2} \\ \mathrm{i}n_2 & 0 \end{bmatrix}\cdots\begin{bmatrix} 0 & \frac{\mathrm{i}}{n_2} \\ \mathrm{i}n_2 & 0 \end{bmatrix}\begin{bmatrix} 0 & \frac{\mathrm{i}}{n_1} \\ \mathrm{i}n_1 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ n_g \end{bmatrix}, \quad \frac{j}{2}=N, \tag{4}$$

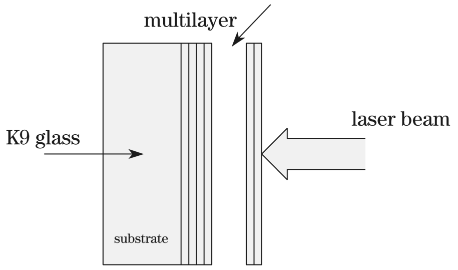

Fig. 1. Structure of the film.

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$$Y_j = C_j/B_j,$$

$$\mathrm{Re}\left(Y_j\right) = \begin{cases} \dfrac{n_g}{\mathrm{A}^2\cos^2\delta + \dfrac{n_g^2}{n_1^2\mathrm{A}^2}\sin^2\delta}, \dfrac{j+1}{2} = N, \\ \dfrac{n_g}{\dfrac{n_1^2}{n_2^2}\mathrm{A}^2\sin^2\delta + \dfrac{n_g^2}{n_1^2\mathrm{A}^2}\cos^2\delta}, \dfrac{j}{2} = N. \end{cases} \tag{5}$$

According to the expression of Poynting vector $\mathbf{I}=\frac{1}{2}\mathrm{Re}\left(E \cdot H^*\right)$, the incidence of light intensity could be expressed as

$$\frac{1}{2}\mathrm{Re}\left(E \cdot H^*\right) = \frac{1}{2}\eta_0 \mathrm{Re}\left(Y\right)\left|E^2\right|, \tag{6}$$

where η_0 is the free space optical admittance, Y is the combined optical admittance of multilayer. The light intensity is

$$I_g = \frac{1}{2}\mathrm{Re}\left(E_g \cdot H_g^*\right) = \frac{1}{2}\eta_0 n_g \left|E_g^2\right|. \tag{7}$$

Electric intensity of any reference plane of the film could be expressed as

$$E_j = \left[\frac{\mathrm{T}}{0.5\eta \mathrm{Re}\left(Y_j\right)}\right]^{1/2}. \tag{8}$$

The light intensity of any reference plane is $I_j = \gamma\left|E_j\right|^2$. The intensity of the light meets Gauss distribution along the direction of radius and $I = I_0 \exp\left(-\dfrac{2r^2}{r_0^2}\right)$, where I_0 is the peak intensity of the light, r_0 is the light spot radius. $Q_j = \alpha_j I_j$, where Q_j is the heat generation of any reference plane, α_j is the absorption coefficient of any reference plane.

During the irradiation, the absorbed light energy is transferred into the heat energy in the films, which obeys the equation of heat conduction as

$$C_i\rho_i\frac{\partial T\left(r,z,t\right)}{\partial t} = \kappa\left[\frac{\partial^2 T\left(r,z,t\right)}{\partial r^2} + \frac{1}{r}\frac{\partial t}{\partial r} + \frac{\partial^2 T\left(r,z,t\right)}{\partial z^2}\right] + Q_j\left(r,z,t\right). \tag{9}$$

The initial condition of the equation is $T\left(r,z,0\right) = T_0$. The boundary condition of the equation is $-\kappa\dfrac{\partial T}{\partial n}\Big|_{r=r_s} = 0$. And C_i and ρ_i are the specific heat and density of the layer of the multilayer, respectively.

The thermal-elastic equation is described as

$$\frac{\partial\sigma_{\mathrm{z}}}{\partial z} + \frac{\partial\sigma_{\mathrm{rz}}}{\partial r} + \frac{\sigma_{\mathrm{rz}}}{r} = 0, \tag{10}$$

$$\frac{\partial\sigma_{\mathrm{r}}}{\partial r} + \frac{\partial\sigma_{\mathrm{n}}}{\partial z} + \frac{\sigma_{\mathrm{r}} - \sigma_\theta}{r} = 0. \tag{11}$$

The constitutive relationship of the multilayer are expressed as follows:

$$\sigma_{\mathrm{r}} = \frac{X}{1+\nu}\left(\frac{\nu}{1-2\nu}\mathrm{e} + \varepsilon_{\mathrm{r}}\right), \tag{12}$$

$$\sigma_{\mathrm{z}} = \frac{X}{1+\nu}\left(\frac{\nu}{1-2\nu}\mathrm{e} + \varepsilon_{\mathrm{z}}\right), \tag{13}$$

$$\sigma_\theta = \frac{X}{1+\nu}\left(\frac{\nu}{1-2\nu}\mathrm{e} + \varepsilon_\theta\right), \tag{14}$$

$$\sigma_{\mathrm{rz}} = \frac{X}{1+\nu}\left(\frac{\nu}{1-2\nu}\mathrm{e} + \varepsilon_{\mathrm{rz}}\right). \tag{15}$$

The geometric deformation relationship of the multilayer are described as

$$\varepsilon_{\mathrm{r}} = \frac{\partial u_{\mathrm{r}}}{\partial \mathrm{r}} + \alpha\left(T - T_0\right), \tag{16}$$

$$\varepsilon_{\mathrm{z}} = \frac{\partial u_{\mathrm{z}}}{\partial \mathrm{z}} + \alpha\left(T - T_0\right), \tag{17}$$

$$\varepsilon_\theta = \frac{u_{\mathrm{r}}}{\mathrm{r}} + \alpha\left(T - T_0\right), \tag{18}$$

$$\varepsilon_{\mathrm{rz}} = \frac{\partial u_{\mathrm{r}}}{\partial \mathrm{z}} + \frac{\partial u_{\mathrm{z}}}{\partial \mathrm{r}}, \tag{19}$$

where $\sigma_{\mathrm{r}}\big|_{r=\mathrm{r_s}} = 0$, $u_{\mathrm{z}}\big|_{r=\mathrm{r_s},z=0} = 0$, bulk strain $e = \varepsilon_{\mathrm{r}} + \varepsilon_\theta + \varepsilon_{\mathrm{z}}$ and body stress $\Theta = \sigma_{\mathrm{r}} + \sigma_\theta + \sigma_{\mathrm{z}}$ meets the equation $e = ((1-2\nu)/X)\Theta$, where σ, ε, u stand for stress, strain, and displacement, respectively. X is Young's model of each layer, ν is the Poisson's ratio.

Finite element method (FEM) is applied to calculate the thermal and the stress distribution of the film. The parameters of films and substrate are shown in Table 1. The thermal-stress of $\mathrm{HfO_2/SiO_2}$ film radiated by a laser at 1064 nm under single pulse mode is simulated. The power of the laser is 50 J/pulse, the duration is 1 ms, and the energy distribution of the light spot obeys the Gauss distribution. The spot radius of laser is 1 μm, and the peak power of the light is 3.2×10^{10} W/m^2[10].

Figure 2 shows the distribution of electric field intensity along the direction of the depth of the film. From Fig. 2, it is found that the electric field intensity of $\mathrm{HfO_2/SiO_2}$ film decreases along the direction of the depth of the film, which shows a typical standing-wave field distribution.

Figures 3 and 4 show the temperature and the stress of upper layer along the radial direction, respectively. The temperature decreases from 420 K at the spot center to 316 K at the periphery. The stress decreases from 140 MPa at the spot center to 30 MPa at the periphery. It is obviously that the stress as well as the temperature of the upper layer decreases along the radial direction.

Table 1. Optical and Thermal Physical Properties of Multilayer[7]

Layer	Refractive Index n	Extinctive Coefficient	Specific Heat J/(kg · K)	Heat Conductivity (W · K)/m	Young's Model (GPa)	Possion's Ratio	Thermal Expansion ($\times 10^{-6}$ K^{-1})
G (glass)	1.52	10^{-7}	774	1.5	81	0.208	8.6
H (HfO_2)	1.985	3×10^{-5}	480	2.0	240	0.243	5.6
L (SiO_2)	1.465	1.2×10^{-5}	841	1.19	87	0.16	0.5

We could get that the stress at the spot center is higher than that at any other positions. It is concluded that the spot center is likely to be destroyed firstly during the irradiation.

Figure 5 shows the temperature distribution along the axial direction. The temperature decreases from 420 K at the upper layer to 407 K at the bottom layer slightly, while the electric intensity distribution at the spot center decreases rapidly. As is described in Fig. 2, the total thickness of the film is about 4 μm, and the radius of the laser spot is 100 μm. So the heat energy conducts from the upper layer to the bottom layer during the irradiation easily. Most of the heat energy at the spot center could not conduct to the margin area in 1 ms. So the difference between the electric intensity distribution and the temperature distribution can be explained.

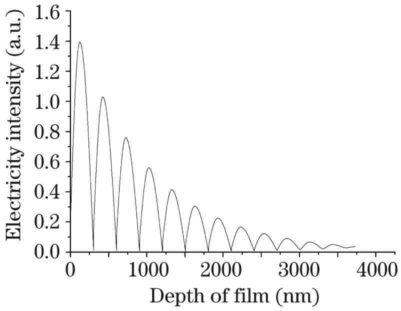

Fig. 2. Normalized electricity intensity at the direction of the depth of film under 1064-nm laser irradiation.

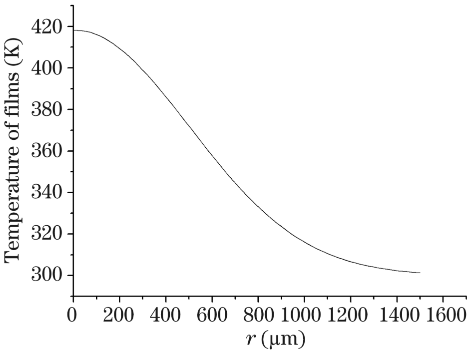

Fig. 3. Temperature distribution along the radial direction of the top layer.

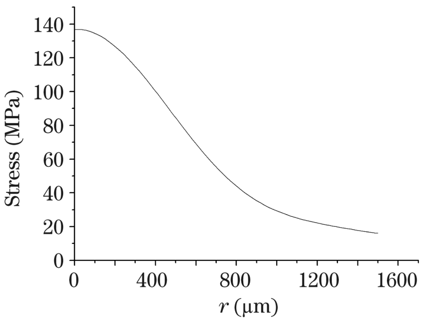

Fig. 4. Thermal-stress distribution along the radial direction of the top layer.

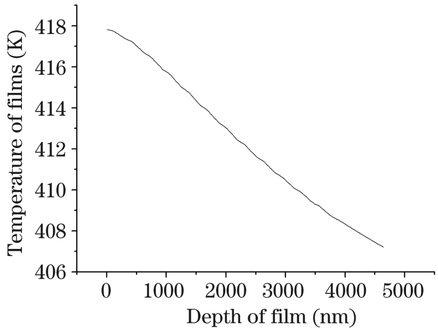

Fig. 5. Stress along the direction of depth of film at the spot center.

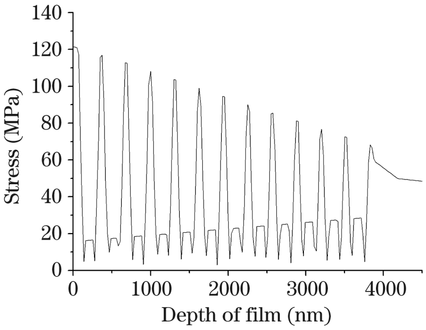

Fig. 6. Temperature along the direction of depth of film at the spot center.

Figure 6 shows the stress along the direction of depth of the film at the spot center. We can get that the stress of HfO_2 layer is much higher than that in SiO_2 layer and the stress in HfO_2 layer decreases along the direction of depth, but the stress in SiO_2 layer increases along the direction. As the absorption coefficient in HfO_2 layer is two times higher than that in SiO_2 layer, and the thermal conductivity of HfO_2 is ten times higher than that of SiO_2, which lead to the stress mismatch of the layer. We could get that the HfO_2 layers are likely to be destroyed firstly during the irradiation.

In conclusion, the thermal stress of HfO_2/SiO_2 film under millisecond laser irradiation is investigated. It is found that the electric intensity pattern plays an important part in the distribution of films. The spot center and the upper layer of HfO_2 layer are likely to be destroyed firstly. The stress mismatch is the main reason of the damage behavior during the high energy long pulse laser irradiation.

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