Wave Interference Effect in Thin Film Structures under Pulsed Laser Irradiation

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The present article conducts extensive numerical simulations to investigate conduction and radiation heat transfer characteristics in thin silicon layers irradiated by pulsed lasers. The two temperature model is used for estimating carrier and lattice temperatures during laser irradiation. The energy absorption in thin films is predicted by the electromagnetic theory, including wave interference effects through thin film optics. The present study predicts the carrier and lattice temperatures during laser irradiation and examines the influence of film thickness and laser pulse duration on characteristics of energy transport. It is observed that, unlike bulk materials, the variation of the film thickness causes significant changes in the reflectivity of silicon film due to wave interference effects in thin film structures. The maximum value of the reflectivity is estimated to be about seven times larger than the minimum value. For the spatial distributions of carrier and lattice temperatures, it is found that a periodic tendency appears for picosecond pulse because of the difference between the pulse duration and the time for energy diffusion. It indicates that the traditional usage of Beer’s law is not appropriate for prediction of radiation heat transfer in thin film structures.

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1. Introduction

In recent years, the interaction of pulsed lasers with solid matter has been one of the most rapidly developing fields in the physical sciences, with wide applications in the semiconductor industry. In particular, the difference in optical characteristics between bulk materials and thin film structures is significant. The energy transport mechanism and optical characteristics of thin film structures under pulsed laser irradiation are rather complicated as compared to those of bulk material. Therefore, it is important to investigate and identify the effects of pulse duration on the energy transport mechanism in thin films.

During transient heating by pulsed laser irradiation, the complex refractive index of materials varies due to changes in temperature and variations in carrier density. These changes can modify the reflectivity and the energy absorption profile, affecting the temperature distributions in thin film structures. Furthermore, the reflectivity of a thin film structure varies significantly with a change in film thickness due to wave interference. This substantial variation of reflectivity plays an important role in determining the amount of energy absorbed in films. In addition, when the film thickness is the same order of magnitude as the phonon mean free path, reduced thermal conductivity from the bulk specimen\textsuperscript{1,2} will occur due to scattering of phonons at the film/substrate interfaces. It is argued in this case that the conventional Fourier law absolutely fails to predict the conductive heat transfer. Therefore, the present study considers nanoscale phenomena such as wave interference, reduction of thermal conductivity, and nonequilibrium between electrons and phonons.

Furthermore, some important parameters such as carrier density, and lattice and carrier temperatures, which are closely connected to one another during pulsed laser irradiation, are very difficult to measure experimentally since the length and time scales are usually much smaller than micrometers and picoseconds, respectively. Computational modeling offers a promising alternative to obtain useful information on the transient temperature fields and the optical characteristics in thin film structures. Grigoropoulos et al.\textsuperscript{3) considered the changes in complex refractive indices of materials by using thin film optics. They showed that utilization of thin film optics in a rigorous manner was essential for both the prediction of the temperature distribution in the irradiated semiconductor material and the development of optical diagnostic methods at the nanosecond scale. However, their model was restricted to pulses with a nanosecond duration. Recently, Moon et al.\textsuperscript{4) measured the thermal conductivity of amorphous silicon thin films and discussed the effects of the reduced thermal conductivity on the temperature in thin film structures when irradiated by pulsed lasers. However, their study did not consider a temperature-dependent thermal conductivity. Moreover, it should be noted that the previous studies do not include the effect of the film thickness when calculating the conductive heat transfer. The mechanism of energy transport and the optical characteristics of thin film structures irradiated by pulsed lasers are poorly understood, in spite of the wide application in the semiconductor industry. Thus, the ultimate goal of this study lies in investigating the energy transfer mechanism and the optical characteristics of thin film structures irradiated by pulsed lasers. For the analysis of the mutual interactions among carrier density, carrier temperature, and lattice temperature, this paper uses the two temperature model\textsuperscript{5–8) which is an approximation of the
Boltzmann transport equation. To consider both the wave interference effects and varying complex refractive indices, this study uses the thin film optics method\(^3,9\) that can determine the energy absorption in the target semiconductor material. In addition, the reduced thermal conductivities,\(^10\) which are estimated by the Equation of Phonon Radiative Transfer (EPRT), are used to consider the effects of phonon scattering at interfaces.

2. Mathematical Formulation

When the laser pulse duration is in the sub-nanosecond range, carrier and lattice temperatures are in non-equilibrium states, the carrier density increases substantially, and the reflectivity of the thin film structure changes significantly because of wave interference. To describe the nonequilibrium state in solid matter irradiated by pulsed lasers, the mutual interaction among photons, carriers, and lattice phonons should be investigated.

2.1 Two temperature model

Typically, the laser beam diameter is 100\(\mu\)m wide, whereas the temperature profile penetration is on the order of 1\(\mu\)m. Thus, one dimensional heat transfer can be assumed essentially at the center of the laser. The two-temperature model developed by van Driel\(^6\) is employed here to describe the interactions among photons, electrons, and phonons. First, the carrier density, \(N_C\), can be determined from

\[
\frac{\partial N_C}{\partial t} = -\gamma N_C^3 + \delta(T_C) N_C + G, \quad (1)
\]

where \(\gamma\) indicates Auger recombination coefficient and \(\delta\) means impact ionization coefficient. Assuming that the inter-band absorption coefficient and the two-photon absorption coefficient are constant, the photo-ionization rate in the bulk material can be estimated from the following relationship.

\[
G(x) = \frac{q_{ba}}{\hbar \omega}. \quad (2)
\]

For a wavelength of 0.53 \(\mu\)m, the two photon absorption coefficient is negligible.\(^10\) In eq. (2), the expression of the photo-ionization rate including the laser intensity is intrinsically difficult to account for wave interference effects in thin film structures. As an alternative, the present study determines the photo-ionization rate directly from the electromagnetic theory as follows:

\[
G(x) = \frac{q_{ba}}{\hbar \omega}. \quad (3)
\]

where \(q_{ba}\) is the volumetric radiation heat source resulting from the inter-band absorption, and it represents an energy source resulting from inter-band absorption.

The energy conservation equations for carriers and lattice phonons are established as follows:

\[
\begin{align*}
\frac{\partial U_C}{\partial t} &= \frac{\partial}{\partial x} \left( k_C \frac{\partial T_C}{\partial x} \right) - \frac{3N_C k_B}{\tau_C} (T_C - T_L) + q_{\text{tot}}, \quad (4) \\
\frac{\partial U_L}{\partial t} &= \frac{\partial}{\partial x} \left( k_L \frac{\partial T_L}{\partial x} \right) + \frac{3N_C k_B}{\tau_C} (T_C - T_L), \quad (5)
\end{align*}
\]

where \(\tau_c\) is the carrier-to-phonon energy relaxation time and \(q_{\text{tot}}\) is the radiation heat source resulting from the inter-band absorption and free carrier absorption. The second terms on the right hand side of eq. (4) and eq. (5) indicate the energy exchange between phonons and carriers. The internal energies of the carrier and lattice are described as follows:

\[
\begin{align*}
U_C &= N_C E_g + C_c T_C, \quad (6) \\
U_L &= C_L T_L, \quad (7)
\end{align*}
\]

As shown in Fig. 1, a silicon layer with thickness \(d_f\) is deposited on a fused silica substrate of thickness \(d_s\). The properties of Si and SiO\(_2\) are listed in Tables 1 and 2, respectively.

\[
\begin{align*}
N_C(x < d_f, t) &= 10^{18} \text{m}^{-3}, \quad N_C(x > d_f, t) \equiv 0, \quad (8) \\
T_C(x, 0) &= T_{L,f}(x, 0) = T_0.
\end{align*}
\]

In eq. (8), the initial carrier density of Si layer\(^6\) is \(10^{18} \text{m}^{-3}\). The carrier and lattice temperatures are initially maintained at 300 K. Since the transmitted laser energy across the interface between Si and SiO\(_2\) is not high enough to yield multi-photon ionization, the increase in carrier density due to ionization is negligible in the SiO\(_2\) layer. At this interface, the carrier does not diffuse into the SiO\(_2\) layer since the bandgap energy of SiO\(_2\) is very high, \(\sim 9\) eV.\(^{11}\) Thus, it is assumed that the carrier density in the SiO\(_2\) layer maintains a zero value during laser irradiation.

Equations (1), (4), and (5) are solved to determine \(N_C\), \(T_C\), and \(T_L\), for a given Si film layer. However, for the SiO\(_2\) layer, we only consider eq. (5) without the energy exchange term, \(i.e.,\) namely the transient heat diffusion equation.

\[
\frac{\partial T_C}{\partial x} \bigg|_{x=d_f} = 0. \quad (9)
\]

\[
\frac{\partial T_L}{\partial x} \bigg|_{x=d_f} = 0. \quad (10a)
\]

\[
\frac{\partial T_{L,f}}{\partial x} \bigg|_{x=d_f} = \frac{\partial T_{L,s}}{\partial x} \bigg|_{x=d_f}. \quad (10b)
\]

\[
T_{L,f}(x, t) = \frac{R_{\text{BR}}}{}(T_{L,s}(x = d_s, t) - T_{L,f}(x = d_f, t)). \quad (10c)
\]

At the top surface, the adiabatic condition is applied since the incident laser intensity is sufficiently high such that the

![Fig. 1 The schematic of the Si/SiO\(_2\) thin film/substrate system under pulsed laser irradiation.](image)
convective and radiative heat losses from the top surface can be ignored. Equation (10) represents the boundary conditions at the Si/SiO\(_2\) interface. Unfortunately, at the interface between semiconductor and dielectric materials heated by highly intensive lasers, such a concrete mechanism behind the carrier-phonon interaction has been poorly understood. Similar to the model proposed by Majumdar and Reddy\(^{12}\), the present study considers the energy transport across a highly excited semiconductor and dielectric interface with boundary conditions represented by eq. (10). In eq. (10a), the carrier energy in the Si film layer can not be directly transferred to phonons in the \(\text{SiO}_2\) layer. In eqs. (10b) and (10c), the phonons of the Si film layer transfer their energy to the phonons of the \(\text{SiO}_2\) layer across the interface with a thermal boundary resistance \(R_{\text{BTR}}\). The phonon MFP of silicon\(^{13}\) is about 260 nm. The present study uses the thermal conductivities estimated for different film thicknesses as listed in Table 3, and the thermal boundary resistance is also assumed to be a constant value of \(1.25 \times 10^{-9} \text{m}^2\text{K/W}\) estimated by Kang.\(^{10}\)

### 2.2 Radiation models

#### 2.2.1 Dielectric functions

The complex dielectric function which is closely associated with the complex refractive index \((\hat{n} = n - ik = \sqrt{\varepsilon})\) can be modeled\(^{14}\) using two a summation of independent contributions to the complex dielectric function as follows:

\[
\hat{\varepsilon} = \hat{\varepsilon}_\text{Si} = \left( \frac{\omega_p}{\omega} \right)^2 \frac{1}{1 + \frac{1}{\omega \tau_\text{D}}}.
\]  

(12)

where \(\hat{\varepsilon}_\text{Si}\) is the temperature dependent dielectric constant of unexcited crystalline silicon, and \(\omega_p\) is the plasma frequency. The damping time, \(\tau_\text{D}\) is assumed to be 1.0 fs when considering carrier-carrier collisions.\(^{15}\) The second term is considered the Drude response of laser-generated free electrons.\(^{14}\) The temperature-dependent dielectric function is obtained from the temperature-dependent complex refractive index\(^{16,17}\) which is listed in Table 1. The plasma frequency \(\omega_p\) is expressed as

\[
\omega_p = \left( \frac{N_e e^2}{\varepsilon_0 m^* m_e} \right)^{\frac{1}{2}},
\]

(13)

where \(m^*\) is the ratio of electron effective mass to rest mass,\(^{14}\) assumed to be 0.18.

#### 2.2.2 Thin film optics

In this study, the electromagnetic theory is used to consider the wave interference effect and spatial change in the refractive index during laser irradiation. In order to estimate the spatial change in optical constants, the present study divides the thin film structure into several grids as seen in Fig. 2. Using the formalism of the characteristic transmission

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**Table 1** Physical properties of silicon.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat capacity of the carrier, (J m^{-3} K^{-1})</td>
<td>(C_C = 3 N_e k_B)</td>
</tr>
<tr>
<td>Heat capacity of the lattice, (J m^{-3} K^{-1})</td>
<td>(C_L = 1.978 \times 10^8 + (3.54 \times 10^8 K^{-1}) T_L - (3.68 \times 10^8 K^2) T_L^{-2})</td>
</tr>
<tr>
<td>Carrier thermal conductivity, (W m^{-1} K^{-1})</td>
<td>(k_C = -0.556 + 7.13 \times 10^{-3} T_C)</td>
</tr>
<tr>
<td>Auger recombination coefficient, (m^3 s^{-1})</td>
<td>(\gamma = 3.8 \times 10^{-43})</td>
</tr>
<tr>
<td>Impact ionization coefficient, (s^{-1})</td>
<td>(\delta = 3.6 \times 10^{-10} \exp(-1.5 E_p/\hbar k T_C))</td>
</tr>
<tr>
<td>Band gap, (\text{eV})</td>
<td>(E_p = 1.86 \times 10^{-19} - 1.12 \times 10^{-22})</td>
</tr>
<tr>
<td>Real part of refractive index of unexcited silicon</td>
<td>(\hat{n}_s = 4.159 + 5.025 \times 10^{-8} (T_L - 300)) (at (\lambda = 0.53) μm)</td>
</tr>
<tr>
<td>Imaginary part of refractive index of unexcited silicon</td>
<td>(k_s = 2.12 \times 10^{-2} \exp(T_L/430)) (at (\lambda = 0.53) μm)</td>
</tr>
<tr>
<td>Electron-lattice scattering rate, (\text{ps})</td>
<td>(\tau_C = 0.5[1 + (N_e/2 \times 10^2)])</td>
</tr>
</tbody>
</table>

**Table 2** Physical properties of \(\text{SiO}_2\).

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice specific heat, (J m^{-3} K^{-1})</td>
<td>(C_L = 2.64 \times 10^8)</td>
</tr>
<tr>
<td>Lattice thermal conductivity, (W m^{-1} K^{-1})</td>
<td>(k = 1.4)</td>
</tr>
<tr>
<td>Real part of refractive index, (n = 1.46) (at (\lambda = 0.53) μm)</td>
<td>(n = 1.46) (at (\lambda = 0.53) μm)</td>
</tr>
<tr>
<td>Imaginary part of refractive index, (k = 0) (at (\lambda = 0.53) μm)</td>
<td>(k = 0) (at (\lambda = 0.53) μm)</td>
</tr>
</tbody>
</table>

**Table 3** Temperature dependent thermal conductivity of thin silicon film for different film thicknesses.\(^{10}\)

<table>
<thead>
<tr>
<th>Film Thickness, nm</th>
<th>Temperature dependent thermal conductivity, (k_L/W m^{-1} K^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>0.221 (10^8 T_L^{-0.978})</td>
</tr>
<tr>
<td>100</td>
<td>0.368 (10^8 T_L^{-1.038})</td>
</tr>
<tr>
<td>190</td>
<td>0.619 (10^8 T_L^{-1.104})</td>
</tr>
<tr>
<td>500</td>
<td>1.028 (10^8 T_L^{-1.172})</td>
</tr>
</tbody>
</table>

---

**Fig. 2** Schematic of the multilayer, stratified structure.
matrix, the lumped structure reflectivity can be obtained. The characteristic matrix of the $m$-th layer with complex refractive index ($\tilde{n}_m = n_m - i k_m$) is given by

$$
M_m = \begin{bmatrix}
\cos\left(\frac{2\pi}{\lambda} \tilde{n}_m d_m\right) & i \tilde{n}_m \cos\left(\frac{2\pi}{\lambda} \tilde{n}_m d_m\right) \\
\tilde{n}_m \sin\left(\frac{2\pi}{\lambda} \tilde{n}_m d_m\right) & \cos\left(\frac{2\pi}{\lambda} \tilde{n}_m d_m\right)
\end{bmatrix},
$$

(14)

The characteristic matrix of the whole medium, considered as a pile of thin layers, is equal to

$$
M = \prod_{m=1}^{N} M_m.
$$

(15)

The reflection and transmission coefficients, $r$ and $t_r$, are

$$
r = \frac{[M(1,1) + M(1,2)\tilde{n}_s\tilde{n}_a] - [M(2,1) + M(2,2)\tilde{n}_a\tilde{n}_s]}{2\tilde{n}_a},
$$

(16)

$$
t_r = \frac{[M(1,1) + M(1,2)\tilde{n}_a\tilde{n}_s] + [M(2,1) + M(2,2)\tilde{n}_s\tilde{n}_a]}{2\tilde{n}_a}.
$$

(17)

Finally, the structure reflectivity and transmissivity in terms of $r$ and $t_r$ can be described as

$$
R = \frac{|E_s|^2}{|E_s|^2} = |r|^2,
$$

(18)

$$
\tau = \frac{n_a|E_a|^2}{n_s|E_s|^2} = \frac{n_s}{n_a} |t_r|^2.
$$

(19)

### 2.2.3 Laser energy absorption in thin film structures

Typically, the laser intensity can be represented by the Gaussian pulse as follows:

$$
I(x = 0, t) = I_0(1 - R(t)) \exp\left(-4.0(\ln 2) \frac{t^2}{t_p^2}\right),
$$

(20)

where $I_0$ represents the maximum intensity given by

$$
I_0 = \frac{2F}{\sqrt{\pi} \ln 2t_p}.
$$

(21)

Because this study considers the nonuniform distributions in space and time, the spatial distribution of the laser intensity is very important. In bulk semiconductors, the spatial gradient of laser intensity is written as follows:

$$
\frac{d}{dx} I(x, t) = -\alpha I - \beta I^2 - \Theta N e I.
$$

(22)

It is noted that for a low intensity and short wavelength laser, the two-photon absorption is negligible, whereas at the high intensities, the free carrier generation via two-photon absorption is dominant in the silicon. Equation (22) representing Beer’s law is suitable for bulk materials where laser intensity attenuates exponentially. However, in nanoscale thin film structures, the laser intensity does not decay exponentially due to the interference of waves. In that case, the use of electromagnetic theory provides an alternative to estimate the laser intensity distribution in a more rigorous manner. The model of Grigoropoulos et al. is adopted for the present simulation.

Assuming that the electromagnetic field is periodic in time, with a time dependence $e^{j\omega t}$, Maxwell’s equations for complex electric and magnetic fields vectors become:

$$
\nabla \times \mathbf{H} = io\omega \mathbf{E},
$$

(23)

$$
\nabla \times \mathbf{E} = -i\omega \mu \mathbf{H}.
$$

(24)

A plane wave is incident on the structure with the electric field amplitude, $E^+$. Using plane wave solutions, the corresponding energy flow incident on the structure is obtained as follows:

$$
S = \frac{n_a}{2\mu \varepsilon_c} |E^+|^2 i.
$$

(25)

The electric field amplitudes of the reflected and transmitted waves at the surface, $E_s$ and $E_t$, are obtained from eqs. (18) and (19). Using the electric field amplitudes, the Poynting vectors are determined along the $x$ direction in the $m$-th layer as follows:

$$
S_m(x) = \frac{1}{2\mu \varepsilon_c} \text{Re}\left(\tilde{n}_m \times (E_m^+(x) + E_m^-(x))\right)
$$

$$
\times (E_m^+(x) - E_m^-(x))^*\right),
$$

where

$$
E_m^+(x) = E_m^0 e^{-i\tilde{n}_m(x-x_n)},
$$

(27a)

$$
E_m^-(x) = E_m^0 e^{i\tilde{n}_m(x-x_n)}.
$$

(27b)

The local energy flow is normalized by the energy flux incident on the structure represented in eq. (25) as follows:

$$
S_m(x) = \frac{1}{n_a |E^+_a|^2} \text{Re}\left(\tilde{n}_a \times (E_m^+(x) + E_m^-(x))\right)
$$

$$
\times (E_m^+(x) - E_m^-(x))^*\right).
$$

(28)

The radiation energy absorption in the $m$-th layer can be determined from

$$
q_{tot} = I(0, t) \frac{dS_m}{dx}.
$$

(29)

where $q_{tot}$ involves both inter-band absorption and free carrier absorption. This result is used for solving the carrier energy conservation equation. As seen in eq. (3), however, the photo ionization rate is only related to the inter-band absorption process. Thus, we need a new relationship for $q_{iba}$ to determine the evolution of the carrier density. From the fluctuation dissipation theorem, the real and imaginary parts of a dielectric function are related to both dispersion and absorption. Dispersion indicates that the direction of radiation is altered and both the wavelength and speed of propagation are affected. However, the propagation remains lossless. Absorption indicates that the energy density in the radiation changes as it moves through the medium. Hence, the absorption is proportional to the imaginary part of the dielectric function, and finally $q_{iba}$ can be obtained as follows:

$$
q_{iba} = \frac{\text{Im}(\varepsilon_i)}{\text{Im}(\varepsilon_i)} q_{tot}.
$$

(30)

### 3. Computational Details

All properties are taken to be dependent on the local temperature and carrier density. As shown in Fig. 2, a silicon film is divided into several grids for calculation. Those grids can be regarded as layers when using the radiation model.
From grid and time independence tests, a uniform 100 point grid is used in the silicon film and a non-uniform 100 point grid is used in the substrate. The time step is chosen to be 0.01 $t_p$ for all calculations. Equations (1), (4), and (5) are discretized using the Crank-Nicholson scheme and finite volume method. They are solved simultaneously with the radiation model, considering all variable properties at each time step. The iteration loop for a stable solution is terminated when the relative deviation of each temperature time step. The iteration loop for a stable solution is terminated when the relative deviation of each temperature calculation is less than $10^{-3}$ and the sum of residuals from the energy equations are less than $10^{-3}$. The initial time is set to $t_{\text{init}} = -5t_p$ and the laser wavelength is 530 nm for all cases. It should be noted that the negative value of time is chosen such that $t = 0$ represents the time at which the incident energy has a peak value.

4. Results and Discussion

To examine the influence of wave interference in thin silicon film structures, the present study considers four different thicknesses of thin silicon films, i.e., 50 nm, 100 nm, 190 nm, and 500 nm. For a film thickness normalized to the laser wavelength in the film, $\lambda_f = \lambda/m_f$. Fig. 3(a) shows predicted values of the reflectivity at room temperature. A substantial change in reflectivity can be observed clearly for different film thicknesses. In particular, maximum and minimum values of the reflectivity are apparent for film thicknesses of 100 nm and 190 nm, respectively. The highest value of reflectivity is estimated to be 0.7 and the smallest value to be 0.1. It is clearly seen in Fig. 3(a) that the reflectivity shows periodic pattern with $2d_f/\lambda_f$, due to the wave interference occurring in the film structure. It is believed to play an important role in determining the amount of radiation energy absorbed in thin films.

Figure 3(b) exhibits the temperature effects on reflectivity. In Fig. 3(b), the estimated values of reflectivity are plotted for a film thickness normalized by the laser wavelength, $\lambda$. Since the real part of the refractive index represents the propagation velocity of light through the material, the increase in temperature leads to a decrease in velocity inside the silicon film. In fact, the decrease in velocity can be considered equivalent to a decrease in the wavelength in film, $\lambda_f$. Thus, if the reflectivity is plotted against $d_f/\lambda_f$, the curve shifts towards larger values of $d_f/\lambda_f$, as shown in Fig. 3(b). However, if the reflectivity is plotted against $d_f/\lambda$, all curves lie atop each other. The fact that the reflectivity becomes closer to the bulk value for higher temperatures is due to the increase in the imaginary part of the refractive index, $k_m$. This result indicates that wave interference effects diminish and a rapid increase in energy absorption occurs.

From the results mentioned above, the ratio, $d_f/\lambda_f$, is truly a crucial factor in determining the optical characteristics of thin silicon structures. In other words, the selective determination of film thickness as well as laser wavelength may be important to film characterization. In addition to the film temperature, the present study focuses on the effect of carrier density on the optical characteristics when high intensity laser energy is incident on the layered material. As seen in Fig. 4, the increase in carrier density reduces the real part of refractive index and changes the optical characteristic of thin film structures. When the carrier density is below $10^{25}$ m$^{-3}$, the change in reflectivity becomes small due to the small variation of the real part of the refractive index. On the other hand, for carrier densities higher than $10^{26}$ m$^{-3}$, the real part of refractive index is rapidly changing. In this case, the carrier density effects on the optical characteristics become important.

In order to examine the influence of film thickness on the optical characteristics, the present study uses a laser wavelength of 530 nm and the laser fluence of 500 J/m$^2$ K for two different laser pulse durations, 10 ns and 20 ps. Figure 5 presents the transient behavior of the reflectivity at the top surface for different film thicknesses for the 10 ns pulse. At $t = -t_p$, the values of reflectivity should be same as those obtained from the thin film optics seen in Fig. 3(a). The reflectivities estimated for layer thicknesses of 50 nm and 100 nm remain almost constant during laser irradiation. This characteristic is caused by a high reflectivity which decreases the surface absorption of laser energy, resulting in a rise of lattice temperature much smaller than the cases with layer thicknesses of 190 nm and 500 nm.

![Fig. 3](image-url) (a) The influence of the ratio $d_f/\lambda_f$ on estimated reflectivities, and (b) the temperature effects on reflectivity; for all cases, $\lambda = 0.53$ μm.
In Fig. 6, the carrier density when layer thickness is \(d = 190\) nm is the largest among those studied, whereas the film thickness of 100 nm exhibits the smallest carrier density. In general, when the reflectivity is smaller and the energy absorption is larger, a higher carrier density will occur. This pattern is closely associated with the transmitted laser energy at the top surface, which is determined by the reflectivity. It is also noted that the increased carrier density for a pulse duration of 10 ns is below \(10^{26}\) m\(^{-3}\), with an associated small effect on the optical characteristics. For the 20 ps pulse, however, the carrier density appears to be higher than \(10^{26}\) m\(^{-3}\) and its influence on the optical characteristics is obviously large.

For the laser pulses of 10 ns and 20 ps, the estimated carrier and lattice temperatures at the top surfaces are presented in Fig. 7. For the 10 ns pulse, a similar tendency is found between carrier and lattice temperatures since the laser pulse duration is much longer than the relaxation time between carrier and phonon. It means that, at \(t_p = 10\) ns, the carrier and lattice temperatures are in thermal equilibrium. The rise of the lattice temperature is closely connected with the variation of the reflectivity, and is substantially affected by the amount of laser energy absorbed in materials. For instance, as seen in Figs. 3(a) and 5, when the reflectivity is the smallest at \(d = 190\) nm, the laser energy absorption is the largest, which allows carrier and lattice temperatures to approach their maximum values. This feature is a result of the increase in the lattice temperature, which in turn produces an increase of the imaginary part of the complex refractive index, leading to a larger absorption of laser energy. For the \(t_p = 20\) ps pulse, there is a quite different behavior from the case of the 10 ns pulse, indicating that the carrier temperature changes drastically with film thickness. It also exhibits two peaks as a function of time; the first peak is due to direct laser heating of the carriers and the second peak is present due to Auger heating, as mentioned by van Driel.\(^{50}\) In addition, as opposed to the 10 ns laser pulse, substantial nonequilibrium between carriers and lattices is clearly observed due to a difference between the energy relaxation time and the pulse duration.
Figure 8 illustrates the spatial distribution of the energy absorption with periodic behavior due to wave interference, which intrinsically appears in thin film structures. The $x$ axis is defined as the dimensionless distance obtained by dividing the distance from a Si/SiO$_2$ interface to the top surface by the wavelength in film, $\lambda_f$. It is interesting to note that the spatial distributions of absorption for all cases show similar patterns for the same wavelength although the magnitude of energy absorption might be different due to different values of the reflectivity. It should also be noted that the period of the absorption patterns is equal to $1/\lambda_f = 2$ since electromagnetic waves with a pattern of $\exp(ik_m x)$ have an interference energy flux or absorption of $\exp(i2k_m x)$. For nanosecond-to-picosecond laser pulses, such wave-like behaviors seem to exist and they support that the traditional Beer’s law in laser applications fails to predict radiation heat transfer in thin film structures.

Figure 9 represents spatial distributions of carrier and lattice temperatures, such as the periodic tendency found for the 20 ps pulse, but not observed for the 10 ns pulse. This aspect arises since the laser pulse duration is too short relative to the time for energy diffusion in case of the 20 ps pulse.
The fact that the diffusion coefficient of the lattice phonon is larger than that of the carrier means that the lattice energy diffuses much faster than the carrier energy. This difference between two diffusion coefficients makes the periodic pattern in carrier temperature more clear. The periodic temperature profiles in Figs. 9(c) and 9(d) confirm that the traditional Beer’s law based on the exponential decay of optical absorption in bulk materials cannot be used for the prediction of radiation heat transfer in thin film structures when the optical absorption depth is longer than film thickness. Thus, the use of thin film optics and the reduced thermal conductivity would be indispensable in predicting temperature distribution in the semiconductor material as well as in developing optical diagnostic methods.

5. Conclusions

The present study investigated the energy transfer mechanism and optical characteristics of thin film structures irradiated by pulsed lasers. The conclusions were drawn as follows.

Due to wave interference, as opposed to the bulk material, the reflectivity of a silicon thin film structure is highly affected by film thickness. The maximum reflectivity of a thin silicon film is about seven times larger than the minimum reflectivity. Thus, the reflectivity becomes very important for the determination of the amount of radiation energy absorbed in thin films. For nanosecond pulse lasers, the spatial absorption distributions appear periodic, whereas the influence of wave-like patterns on radiation energy absorption can be ignored for carrier and lattice temperatures. On the other hand, for picosecond pulse lasers, spatial carrier and lattice temperature distributions show clear periodic tendencies because the pulse duration is shorter than the time for energy diffusion. In particular, the appearance of wave-like behavior clearly supports that the traditional Beer’s law in laser applications cannot be used for the prediction of radiation heat transfer in thin film structures. It is concluded that the thin film optics and the reduced thermal conductivity should be considered when investigating laser-solid interactions for semiconductor thin film structures heated by short pulse lasers.

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REFERENCES


Appendix

\[ C = \text{heat capacity per unit volume, } J/m^3 K \]
\[ c = \text{speed of light, } 3.0 \times 10^8 m/s \]
\[ d = \text{layer thickness, } m \]
\[ d_s = \text{substrate thickness, } m \]
\[ E = \text{magnitude of electric field vector, } V/m \]
\[ E_g = \text{band gap energy, } J \]
\[ E = \text{electric field vector, } V/m \]
\[ e = \text{electron charge, } C \]
\[ F = \text{laser fluence, } J/m^2 \]
\[ G = \text{photo ionization rate, } 1/m^3 s \]
\[ H = \text{magnetic field vector, } T/m \]
\[ h = \text{reduced Planck constant, } 1.0546 \times 10^{-34} \text{ Js} \]
\[ I = \text{laser intensity, } W/m^2 \]
\[ I_0 = \text{maximum laser intensity, } W/m^2 \]
\[ i = \text{imaginary unit} \]
\[ k = \text{imaginary part of complex refractive index} \]
\[ k_B = \text{Boltzmann constant, } 1.38066 \times 10^{-23} J/K \]
\[ k_C = \text{carrier thermal conductivity, } W/mK \]
\[ k_L = \text{lattice thermal conductivity, } W/mK \]
\[ k = \text{complex wave number} \]
\[ M = \text{characteristic transmission matrix} \]
\[ m_e = \text{electron mass, } kg \]
\[ m^* = \text{ratio of electron effective mass to rest mass} \]
\[ N_C = \text{carrier density, } 1/m^3 \]
\[ n = \text{real part of complex refractive index} \]
\[ n = \text{complex refractive index} \]
\[ q = \text{radiation heat source, } W/m^3 \]
\[ R = \text{Fresnel reflectivity} \]
\[ R_{TBR} = \text{thermal boundary resistance} \]
\[ r = \text{Fresnel reflection coefficient} \]
\[ S = \text{magnitude of Poynting vector, normalized with the incident energy flux} \]
\[ S = \text{Poynting vector, } W/m^2 \]
\[ T = \text{temperature, } K \]
\[ t = \text{time, } s \]
\[ t_0 = \text{pulse duration, } s \]
\[ t_r = \text{transmission Fresnel coefficient} \]
\[ U = \text{energy density, } W/m^3 \]
\[ x = \text{spatial axis, } m \]

Greek
\[ \alpha = \text{linear absorption coefficient, } m^{-1} \]
\[ \beta = \text{two photon absorption coefficient, } m/W \]
\[ \delta = \text{impact ionization coefficient, } s^{-1} \]
\[ \varepsilon_0 = \text{permittivity constant, } 8.85 \times 10^{-12} \text{ C}^2/\text{Nm}^2 \]
\[ \kappa = \text{complex dielectric function} \]
\[ \gamma = \text{Auger recombination coefficient, } m^6/s \]
\[ \lambda = \text{laser wavelength, } m \]
\[ \mu = \text{magnetic permeability, } \text{Tm/A} \]
\[ \Theta = \text{free carrier absorption coefficient, } m^2 \]
\[ \tau = \text{transmissivity} \]
\[ \tau_c = \text{scattering time, } s \]
\[ \tau_d = \text{damping time, } s \]
\[ \omega = \text{angular frequency of laser, rad/s} \]

Subscripts
\[ a = \text{ambient} \]
\[ C = \text{carrier} \]
\[ f = \text{film} \]
\[ iba = \text{interband absorption} \]
\[ L = \text{lattice} \]
\[ m = \text{m-th layer} \]
\[ o = \text{ambient} \]
\[ p = \text{plasma} \]
\[ s = \text{substrate} \]
\[ Si = \text{silicon} \]
\[ tot = \text{total absorption} \]

Superscripts
\[ + = \text{forward wave propagation along the direction of incident laser light} \]
\[ – = \text{reflected wave propagation} \]
\[ * = \text{complex conjugate} \]
\[ 1 = \text{forward wave propagation along the direction of incident laser light} \]
\[ 2 = \text{reflected wave propagation} \]