Optical Characteristics and Nanoscale Energy Transport in Thin Film Structures Irradiated by Nanosecond-to-Femtosecond Lasers

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Extensive numerical simulations are rigorously conducted for conductive and radiative heat transfer characteristics in thin silicon structures irradiated by nano-to-femtosecond pulsed lasers. The two-temperature model is used to calculate the carrier and lattice temperatures, respectively. The wave interference effects on reflectivity and absorption are considered by using the thin film optics and the electromagnetic theory. The radiation property of silicon is expressed in terms of lattice temperature and carrier density. The reflectivity of thin film structures irradiated by femtosecond laser shows very different features with the variation of laser pulse durations. In femtosecond laser irradiation, the energy transfer between carriers and lattice phonons mostly takes place after laser irradiation is over and then it rapidly heats the ions to much higher temperatures, compared to the long pulse cases. For nanosecond pulse lasers, the carrier and lattice temperature distributions do not show wavy patterns, whereas for subpicosecond pulse lasers, the spatial carrier and lattice temperature distributions appear to be periodic in space because of shorter pulse duration than diffusion time. [doi:10.2320/matertrans.MB200820]

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1. Introduction

Generally, lasers have been widely used for material modification and micromachining since their invention more than four decades ago. In material modification with pulsed laser, laser-matter interaction shows very different features with the variation of laser parameters such as kind of material, pulse width, wavelength, and fluence. It is well known that the ultrashort duration of pulse shorter than 10 ps changes the laser-matter interaction mechanisms fundamentally in some aspects. Among laser-matter interaction applications, the thin film structure is one of the most important configurations in semiconductor industry. The energy transport mechanism and optical characteristics of thin film structure under pulsed laser irradiation are rather complicated than those of bulk material due to the small thickness of film. Therefore it is very meaningful to investigate the effects of pulse duration on the energy transport mechanism in laser-thin film structure interaction.

In laser-thin film structure interaction, carrier density, and lattice and carrier temperatures are very important parameters, which are closely connected to one another during rapid irradiation of pulsed lasers. However, it is very difficult to measure them experimentally because the considered scales of length and time are usually smaller than micrometers and picoseconds, respectively. The computational modeling offers a promising alternative to obtain detailed information on the nanoscale energy transfer characteristics in laser-thin film interactions. However, because of small thickness of thin film and short pulse duration of laser, the conventional heat transfer simulation tool fails to analyze such cases. Hence, for the accurate modeling of temperature field and optical characteristic of thin film structures under irradiation of pulsed laser, the present study considers some important nanoscale phenomena such as wave interference, reduction of thermal conductivity, and nonequilibrium between electrons and phonons.

In fact, the energy transport mechanism in dielectric and semiconductor targets under ultrashort pulsed laser irradiations is very complex. This topic has been uncovered thoroughly. As was mentioned previously, it is difficult to measure the carrier densities and the lattice temperatures directly. For this reason, the numerical models may be useful in analysis of micro/nanoscale energy transport in materials. For numerical analysis, hydrodynamic equations are widely used, which are based on Boltzmann transport equation (BTE). Qui and Tien1,2) performed numerical simulations on the interactions between carriers and lattices by simplifying the scattering terms in the BTEs through the quantum analysis. They showed that the excited carriers were no longer in thermal equilibrium with the other carriers, creating a nonequilibrium heating situation, when the laser pulse width was shorter than approximately five times the electron energy relaxation time. Driel3) reported the kinetics of high-density plasmas generated in silicon by picosecond laser pulses with two different wavelengths, and he found that carrier temperature exhibited two peaks as a function of time due to laser heating as well as Auger heating; he explained the interactions among the carrier density, and carrier and lattice temperature. However, Driel’s work did not involve any information on the effect of laser pulse duration on the heat transfer characteristics because it presented predictions only at the fixed laser pulse of 20 ps. Bulgakova et al.4) investigated fast electron transport theoretically based on the drift-diffusion approach for different types of material under ultrafast pulsed laser irradiation. Their simulations were performed in the ablation regime where laser intensities are above the material removal threshold. They reported that a strong electrostatic ion repulsion force causes the breakup of the surface of charged dielectric materials, whereas for semiconductors and metals, the efficient neutralization occurs and ablation receives a more thermal appearance.
Even though the intensive previous works of many researchers, most of them are concerned to bulk materials not to thin film structures. Moreover, the effects of changes in pulse duration on energy transport mechanism are not thoroughly investigated.

The present study aims ultimately to investigate the energy transport mechanism and the optical characteristics of thin film such as reflectivity, absorption under femtosecond to nanosecond pulsed laser irradiation. In particular, this study is devoted to examine wave interference effects on reflectivity and pulse duration effects on energy transport mechanism. It is expected that the present study is useful in designing and diagnosis of semiconductor processing for a variety of industrial applications.

2. Mathematical Representation

In subpicosecond laser heating systems and high-filed electronic devices, nonequilibrium microscale energy transfer between energy carriers and lattice phonons need to be considered. The electron-phonon scattering time scale is on the order of 100 fs in most metals and semiconductors, whereas the phonon-phonon scattering time is on the order of 10 ps. For picosecond to femtosecond laser heating of solids, electrons are in non-equilibrium with the lattice, necessitating the user of multiple step energy transfer models. In other words, carrier density, carrier temperature, and lattice temperature should be determined in a separate way and their interactions needs to be modeled. Another difficulty in analyzing thin film structure is as follows: Thin films are known to exhibit reduced thermal conductivity from bulk specimens due to the scattering of phonons at the film/substrate interface in thin films, when the film thickness approaches the same order of magnitude as phonon mean free path (average distance a heat carrier travels before each collision and thus loss of energy: MFP). In addition, the wave interference occurs due to very small film thickness, compared to laser wavelength. The reflectivity of thin film varies significantly with the change of film thickness compared to laser wavelength. The reflectivity of thin film wave interference occurs due to very small film thickness, collision and thus loss of energy: MFP). In addition, the path (average distance a heat carrier travels before each collision at the center of the substrate interface in thin films, when the film thickness compared to laser wavelength). The reflectivity of thin film structure is as follows: Thin films are known to exhibit reduced thermal conductivity from bulk specimens due to the scattering of phonons at the film/substrate interface in thin films, when the film thickness approaches the same order of magnitude as phonon mean free path (average distance a heat carrier travels before each collision and thus loss of energy: MFP).

2.1 Two temperature model

To study the multiple step energy transfer among photons, electrons and phonons, the average moments of BTE for all these individual systems are solved simultaneously. Typically, 1/e^2 radii of the laser beams are on the orders of 10–1000 μm, whereas the temperature profile penetrations are on the orders of 0.1–1 μm. Thus, an assumption of one dimensional heat transfer can be made at the center of the laser. In this study, the similar form of Driel’s governing equation is adopted and at first the balance equation for carrier becomes

\[
\frac{\partial N_C}{\partial t} = \frac{\partial}{\partial x} \left( D_C \frac{\partial N_C}{\partial x} \right) + G + R,
\]

where \( D_C \) is carrier ambipolar diffusivity, \( G \) and \( R \) are the pair generation and net recombination rates. The net recombination rate is given by

\[
R = -\gamma N_C^2 + \delta(T_C)N_C,
\]

where \( \gamma \) and \( \delta \) are the Auger recombination and impact ionization coefficients, respectively. With the assumption of constant interband absorption coefficient and two-photon absorption coefficient, the generation rate in bulk material is simply written as follows.

\[
G(x) = \frac{\alpha I}{\hbar\omega} + \frac{\beta I^2}{2\hbar\omega},
\]

where \( \alpha \) is the linear absorption coefficient, \( \beta \) is the two photon absorption coefficient and \( \omega \) is angular frequency of laser. For the wavelength of 0.53 μm which is used in this study, the two photon absorption coefficient is negligible. However, this simple expression for generation rate is not applicable for thin film structure. In thin film structure, the laser intensity shows wavey pattern spatially and does not exponentially decay. Hence, this study takes the following form of generation rate.

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

and the internal energy of carrier is balanced with diffusion energy transfer, energy exchange between carriers and phonons, and energy source from pulsed lasers.

\[
\frac{\partial U_C}{\partial t} = \frac{\partial}{\partial x} \left( k_C \frac{\partial T_C}{\partial x} \right) - \frac{3N_C k_B}{\tau_C} (T_C - T_L) + q_{tot}
\]

where \( U_C \) is the internal energy, \( \epsilon_g \) the band gap energy, \( C_C \) the specific heat, \( k_C \) the conductivity of carrier, \( k_B \) the Boltzmann constant, \( \tau_C \) the carrier-to-phonon energy relaxation time, and \( q_{tot} \) is the total radiation absorption term.

Physically, the second term in RHS means the loss of kinetic energy through equilibration of the lattice and carrier temperatures. As mentioned previously, radiation absorption requires rigorous treatment involving wave interference effect.

The energy conservation equation of lattice phonons can be described as

\[
\frac{\partial U_L}{\partial t} = C_l T_L
\]

where \( k_L \) is the lattice thermal conductivity. The thermal conductivity of thin film is reduced significantly when the thickness of thin film is comparable or smaller than the phonon MFP. The thickness of crystalline silicon thin film
used in this study is 500 nm, and the phonon MFP of silicon is about 260 nm. Kang8) predicted the reduced thermal conductivity and the thermal boundary resistance of thin crystalline silicon films in theoretical ways. These values are used in the present study and listed in Table 1. Equations (1), (6), and (8) determine $N_C$, $T_C$, and $T_L$ completely together with the proper initial and boundary conditions.

2.2 Radiation model

The accurate estimation of reflectivity and absorption profile in space is very crucial in analyzing laser-matter interactions. During laser irradiation, radiation properties are varied because they are substantially affected by carrier number density as well as lattice temperature. Moreover, it is noted that reflectivity and laser absorption in solids is of great dependency on film thickness owing to wave interference. This section introduces some theoretical models to consider the change of radiation property and the wave interference.

2.2.1 Dielectric functions

The dependence of complex refractive index ($\hat{n} = n - ik$) on electron number density and lattice temperature should be understood for determining optical properties of solid matters. Thus, the first step would be to find out the real and imaginary parts of the complex dielectric constant. For silicon, the complex dielectric function can be described on the basis of optical signature of the unexcited material and the Drude response of the laser generated free electron.9)

$$\hat{k} = \hat{k}_{Si} = \left( \frac{\omega_p^2}{\omega} \right)^2 \frac{1}{1 + i \frac{1}{\omega \tau_d}}. \quad (9)$$

where $\tau_d$ is damping time, and $\hat{k}_{Si}$ is a temperature dependent dielectric constant of unexcited crystalline silicon. The damping time is taken 1.1 fs10) considering high carrier-carrier collision. The first term in RHS of eq. (9) is mainly affected by lattice temperature and the second term is varied with excited free carriers. The dielectric constant of unexcited silicon is adopted from Jellison and Modine11) and listed in the Table 1. The plasma frequency $\omega_p$ is expressed as

$$\omega_p = \left( \frac{4\pi N_e e^2}{m^* m_e} \right)^{1/2}, \quad (10)$$

where $m_e$ is the electron rest mass, and $m^*$ is the ratio of electron effective mass to rest mass taken as 0.18.

2.2.2 Reflectivity of thin film structure

When the refractive index is constant and the film is thick enough to ignore wave interference effect, the reflection coefficient for normal incidence at the surface boundary can be easily found from the Fresnel formulas as

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}. \quad (11)$$

The reflectivity is associated with other surface properties such as emissivity and absorptivity through the energy balance.13) Unlike eq. (11), the use of electromagnetic theory would be useful for studying the optical characteristics at the interface between film and substrate. In fact, the electron density and temperature distributions in space lead to drastic change of refractive index.

Along the direction of film depth, a grid system for thin film structure is prepared for examining wave interference characteristics that is varied from temperature and electron number density gradients in space. Using the characteristic transmission matrix,13) the reflectivity and transmissivity of lumped structure is obtained.14,15)

2.2.3 Absorption of radiation energy via pulsed lasers

The variation of laser intensity with time is assumed to follow Gaussian shape as follows:

$$I(x = 0, t) = I_0(1 - R(t)) \exp\left(-4.0(\ln2) \frac{t^2}{\tau_p^2}\right). \quad (12)$$

where $\tau_p$ denotes the laser pulse duration, $R$ is the reflectivity, and $I_0$ represents the maximum intensity given by

$$I_0 = \frac{2F}{\sqrt{\pi} \ln 2 \tau_p}. \quad (13)$$

The present study determines the spatial distributions of laser intensity from the energy balance. In semiconductor, the gradient of laser intensity is written as follows:

$$\frac{d}{dx} I(x,t) = -\alpha I - \beta I^2 - \Theta N_c I, \quad (14)$$

where $\alpha$ indicates linear absorption coefficient, $\beta$ means two-photon absorption coefficient, and $\Theta$ is free carrier absorption coefficient. It is noted that for the case when the laser intensity is relatively low and the wavelength is small, the two-photon absorption is negligible. On the other hand, at high laser intensity, the free carrier generation in silicon is
dominant via the two-photon absorption. Equation (14) indicating Beer’s law is suitable to bulk material where laser intensity is attenuated exponentially. However, in nanoscale thin film structures, the laser intensity no longer undergoes exponential decay because of wave interference. Thus, the present study uses the electromagnetic theory to predict the spatial distribution of laser intensity in more rigorous manner. Assuming that the electric and magnetic fields are periodic in time, with a time dependence $e^{i\omega t}$, Maxwell’s equations for the complex electric and magnetic fields vectors become:

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

(15)

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

(16)

The energy flux along the direction of propagation is given by the time-averaged magnitude of the Poynting vector:

$$\mathbf{S} = \frac{1}{2} \text{Re}(\mathbf{E} \times \mathbf{H}^*)$$

(17)

A plane wave is incident on the structure, with the electric field amplitude, $E_n^i$. The corresponding energy flow along the $x$-direction is:

$$\mathbf{S} = \frac{n_c}{2\epsilon_0} |E_n^i|^2 i.$$

(18)

The electric field amplitudes of reflected and transmitted waves at the surface, $E_n^r$ and $E_n^t$ are obtained using the above expressions. The electric and magnetic fields in the $m$-th layer, $m = 1, \ldots, N$, are given by:

$$E_n^m(x) = E_n^r e^{-ik_m(x-x_n)} + E_n^t e^{ik_n(x-x_n)},$$

(19)

$$H_n^m(x) = \frac{n_c}{\epsilon_0 c} \left[ E_n^r e^{-ik_n(x-x_n)} - E_n^t e^{ik_n(x-x_n)} \right].$$

(20)

where

$$k_m = \frac{2\pi}{\lambda} n_m, \quad x_m = \sum_{j=1}^{m-1} d_j.$$  

(21)

From the continuity of the electric and magnetic fields at each interfaces, the amplitudes of electric fields obtained is:

$$E_n^+(m) = \frac{1}{2} \left( E_{n-1}^+(m-1) \left(1 + \frac{\hat{n}_{n-1}}{\hat{n}_n} \right) e^{-ik_{n-1}d_{n-1}} + \frac{E_{n-1}^-(m-1)}{\hat{n}_n} e^{ik_{n-1}d_{n-1}} \right),$$

(22)

$$E_n^-(m) = \frac{1}{2} \left( E_{n-1}^+(m-1) \left(1 - \frac{\hat{n}_{n-1}}{\hat{n}_n} \right) e^{-ik_{n-1}d_{n-1}} + \frac{E_{n-1}^-(m-1)}{\hat{n}_n} e^{ik_{n-1}d_{n-1}} \right).$$

(23)

Once the amplitudes of electric field at $m-1$-th layer are determined, the amplitudes of electric field at $m$-th layer, $E_n^+$, $E_n^-$, can be obtained recursively. Calculation of the amplitudes $E_n^m$, $E_n^m$, starts from the first layer, where $E_n^+$ and $E_n^-$ are already known, and $d_{m-1} = 0$. From the electric field determined, the Poynting vector is evaluated everywhere in the structure by combining eqs. (24)–(26). In the location $x$ within the $m$-th layer:

$$S_m(x) = \frac{1}{n_c|E_n^m|^2} \text{Re}(E_m(x) \times H_m^*(x)),$$

(24)

or

$$S_m(x) = \frac{1}{2\epsilon_0} \text{Re}(\hat{n}_m)^* (E_m^I(x) + E_m^Q(x))$$

$$\times (E_m^I(x) - E_m^Q(x))^*.\quad (25)$$

where

$$E_m^I(x) = E_m^t e^{-ik_m(x-x_n)},$$

(26)

$$E_m^Q(x) = E_m^t e^{ik_m(x-x_n)}.$$  

(27)

The local energy flow is normalized by the energy flux incident on the structure as follows:

$$S_m(x) = \frac{1}{n_c|E_n^I|^2} \text{Re}(\hat{n}_m)^* (E_m^I(x) + E_m^Q(x))$$

$$\times (E_m^I(x) - E_m^Q(x))^*.$$  

(28)

The absorption in the $m$-th layer is:

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

(29)

Here, $q_{tot}$ means the absorption due to both interband absorption and free carrier absorption. While $q_{iba}$ in the eq. (4) means the absorption due to only interband absorption because eq. (4) is only concerned with carrier density. $q_{iba}$ is obtained from the assumption that $q_{iba}$ is fraction of $q_{tot}$ and can be obtained from following equation:

$$q_{iba} = \frac{1}{\text{Im}(\sqrt{\beta})} q_{tot}.$$  

(30)

3. Numerical Details

As seen in Fig. 1 representing a schematic of computational domain, a silicon film thickness, $d_s$, is deposited on a fused silica substrate with its thickness, $d_f$. Typically, the laser beam diameter is 100 mm wide, whereas the temperature profile penetration is in the order of 1 mm. Thus, the heat transfer at the center of the laser can be assumed to be essentially one dimensional. Transient simulations are conducted using eqs. (1), (6), and (8), and implicit and finite volume methods are used for transient and spatial terms, respectively. The reflectivity of lumped structure is obtained from the characteristic transmission matrix. The radiation absorption profile and the spatial variation of laser intensity are calculated from eqs. (29) and (25), respectively. The initial time is set to $t_{init} = -5t_p$ and the laser wavelength is taken 530 nm for all cases. Here, the negative value of initial time is chosen for convenient analysis of transient phenomena. Because the incident laser intensity considered in this problem is so high, the convective and radiative heat losses from the top surface are negligible. Initially, the carrier and lattice temperatures are maintained at 300 K, and the number density is taken $10^{12}$ cm$^{-3}$. Because of high bandgap energy of SiO$_2$, 9 eV, the carriers in the Si layer does not diffuse in to the SiO$_2$ substrate. Detailed initial conditions and boundary conditions are as follows:

$$N(x, 0) \cong 10^{12} \text{cm}^{-3}, \quad T_L(x, 0) = T_C(x, 0) = T_0.$$  

(31)

$$\frac{dN_C}{dx}_{|x=0} = 0, \quad \frac{dT_C}{dx}_{|x=0} = \frac{dT_L}{dx}_{|x=0} = 0.$$  

(32)
The effects of pulse durations on the optical and energy transfer characteristics of thin film structures are investigated. The pulse durations are varied from 10 ns to 100 fs. For all cases, the film thickness is fixed at 500 nm, and the wavelength and fluence of laser are also given as 530 nm.

The final solutions are obtained when the relative deviation of each temperature is less than $10^{-4}$ and the residuals from energy equations are likewise less than $10^{-3}$. In addition, the values of the parameters used in the simulation are listed in Table 2.

### 4. Results and Discussion

The effects of pulse durations on the optical and energy transfer characteristics of thin film structures are investigated. The pulse durations are varied from 10 ns to 100 fs. For all cases, the film thickness is fixed at 500 nm, and the wavelength and fluence of laser are also given as 530 nm and 0.1 J/m$^2$.

Figure 2 shows the transient behavior of surface reflectivity for different laser pulses. The reflectivities near the early stage of laser irradiation are all the same, because very small amount of laser energy is irradiated. The reflectivity becomes larger as the pulse duration gets shorter. In the long pulse regime, the increase in carrier density is not as high as that in the short pulse regime. Therefore, the complex refractive index is mostly influenced by lattice temperature. On the contrary, in the short pulse regime, the carrier density increases highly for a short time, and consequently the complex refractive index is affected mainly by carrier density. Each role of temperature and carrier density on the complex refractive index is different each other, which results in showing different behaviors of reflectivity with respect to laser pulses. In more detail, at longer pulse duration, temperature effect is dominant in increasing complex refractive index, whereas as pulse duration decreases, carrier density plays an important role in varying optical characteristics.\(^8\)

Figure 3 represents the influence of pulse durations on carrier number densities and carrier temperatures. The increasing tendency in carrier density can be observed as the pulse duration becomes shorter. The carrier density decreases considerably after the end of laser pulse. Nevertheless, it should be noted that the carrier density distribution at 100 fs is different from other cases for longer pulse durations. Although the laser intensity at 100 fs is 10 times higher than that at 1 ps, the peak of carrier density is smaller than that at 1 ps. Once laser pulses are shorter than energy relaxation time between electrons and phonons, the lattice remains cold while laser pulse is being irradiated. Thus, the imaginary part of complex refractive index at 100 fs does not increase as high as the one at longer pulse durations. Because of relatively cold lattice temperature, the energy absorption owing to interband transition becomes smaller, compared to other cases for longer pulses. Another thing to note is that the carrier density does not decrease abruptly, even after the end of pulse duration. This fact is totally distinguished from other cases for longer pulse duration. It is because Auger recombination process does not work at very short pulse durations. It is noted that the carrier temperature distribution has no longer two-peaks for femtosecond laser pulses.\(^8\)

Figure 4 presents the influence of laser pulse on lattice temperature at the front surface. At longer pulse duration, the lattice temperature increases significantly during laser irradiation and it decreases slowly after the end of laser heating. On the other hand, at pulse duration shorter than 10 ps, the lattice temperature increases after irradiation. This difference is due to scale difference between relaxation time and pulse duration. In fact, the carrier-phonon relaxation time is about 0.5 ps in silicon.\(^3\) At a very short pulse, the carrier does not have sufficient time to transfer its energy to lattice phonon for laser pulse duration. Because of the scale difference, the carrier transfers energy to the lattice continuously, even if laser irradiation is terminated. It is true that for femtosecond laser irradiation, the carrier-to-lattice energy transfer takes place mostly after the end of laser pulse, and then it will heat

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**Table 2** Physical properties of SiO$_2$.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice specific heat</td>
<td>$C_L = 2.641$ J/(cm$^2$K)</td>
</tr>
<tr>
<td>Lattice thermal conductivity</td>
<td>$k_L = 1.4 \times 10^{-2}$ W/(cm K)</td>
</tr>
<tr>
<td>Real part of refractive index</td>
<td>$n = 1$ (at $\lambda = 0.53 \mu$m)</td>
</tr>
<tr>
<td>Imaginary part of refractive index</td>
<td>$k = 0$ (at $\lambda = 0.53 \mu$m)</td>
</tr>
</tbody>
</table>

\[ \frac{\partial N_C}{\partial x} \bigg|_{x=d_l} = \frac{\partial T_C}{\partial x} \bigg|_{x=d_l} = 0, \quad k_c = \frac{\delta T_C}{k_{L,f} \delta x_{L} + k_{L,s} \delta x_{s} + R_{TBR}} \quad (33) \]

\[ N_C(x \rightarrow \infty, t) \equiv 10^{12} \text{cm}^{-3}, \]

\[ T_L(x \rightarrow \infty, t) = T_C(x \rightarrow \infty, t) = T_0, \quad (34) \]

The final solutions are obtained when the relative deviation of each temperature is less than $10^{-4}$ and the residuals from energy equations are likewise less than $10^{-3}$. In addition, the values of the parameters used in the simulation are listed in Table 2.

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**Fig. 2** Effects of pulse duration on normal surface reflectivity.
rapidly the ions to much higher temperature, compared to the cases for longer pulses.

Figure 5 illustrates the transient behaviors of carrier and lattice temperatures to show the presence of non-equilibrium between them. At 10 ns, the carrier and lattice temperatures are almost the same. It means the nonequilibrium between the carrier and the lattice temperature does not exist in nanosecond pulse duration and its extent increases as laser pulse decreases.

At 10 ps, the nonequilibrium region is forming during laser irradiation, whereas at 100 fs, the carrier temperature increases substantially compared to the lattice temperature. In particular, it is found that nonequilibrium state at 100 fs persists for a long time after laser irradiation.

Figure 6 represents the spatial distributions of carrier and lattice temperatures at $t = 0.4t_p$. The wavy patterns both in carrier and lattice temperatures are observed at shorter laser pulses more clearly than at longer pulses. It is because of wave interference, indicating that Beer’s law widely used in laser applications does not work any more for a very thin film structure. It is also interesting to note that at 100 ps pulse duration, the lattice temperature distribution has such wavy tendency obviously, whereas those wave-like patterns are not observed clearly for carrier temperature distribution. As a matter of fact, the diffusion coefficient of carrier is larger than that of lattice phonon. This means that the carrier energy diffuses faster than the lattice energy. This difference between two diffusion coefficients makes the wavy pattern more clearly in lattice temperature than carrier temperature.

5. Conclusions

The present study investigated numerically the energy transfer mechanism and the optical characteristics of thin film structures irradiated by nanosecond to femtosecond pulsed lasers. The self-consistent theoretical models based on

Fig. 3 Effects of pulse duration on (a) carrier density and (b) carrier temperature.

Fig. 4 Effects of pulse duration on surface lattice temperature; (a) for $-5t_p < t < 20t_p$ and (b) for $-t_p < t < t_p$.

Fig. 5 Comparison between $T_C$ and $T_L$. 
the BTE are established to characterize the microscale heat transfer mechanism by explaining mutual interactions among carrier density, carrier temperature, and lattice temperature. The two temperature equations are used for calculating semiconductor thin film structures under pulsed laser irradiations. It is emphasized that the optical characteristics in thin film structures are quite different from those in bulk structures due to wave interference as well as scale difference between relaxation time and pulse duration. From the present study, the following conclusions are drawn.

1) The reflectivity of thin silicon film depends highly on lattice and carrier temperatures, carrier density, and pulse duration. At longer pulses, temperature effect becomes dominant in increasing complex refractive index, whereas as pulse duration decreases, the variation of carrier density affects the optical characteristics substantially.

2) In femtosecond laser irradiation, the energy transport between carrier and lattice takes place mostly after the laser irradiation is terminated, and then it heat rapidly the ions to much higher temperatures, compared to long pulse cases.

3) It is found that for nanosecond pulsed lasers, the spatial distributions of both carrier and lattice temperatures do not show wave-like patterns, whereas they show wavy tendencies more clearly because diffusion time would be longer than laser pulse duration. This fact emphasizes that the wave interference effect should be involved for examining microscale energy transfer in thin film structures.

REFERENCES


Fig. 6 Effects of pulse duration on (a) carrier temperature and (b) lattice temperature at \( t = 0.4t_p \).