

Nonequilibrium Heat Transfer Characteristics During Ultrafast Pulse Laser Heating of a Silicon Microstructure

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This work provides the fundamental knowledge of energy transport characteristics during very short-pulse laser heating of semiconductors from a microscopic viewpoint. Based on the self-consistent hydrodynamic equations, in-situ interactions between carriers, optical phonons, and acoustic phonons are simulated to figure out energy transport mechanism during ultrafast pulse laser heating of a silicon substrate through the detailed information on the time and spatial evolutions of each temperature for carriers, longitudinal optical (LO) phonons, acoustic phonons. It is found that nonequilibrium between LO phonons and acoustic phonons should be considered for ultrafast pulse laser heating problem, two-peak structures become apparently present for the subpicosecond pulses because of the Auger heating. A substantial increase in carrier temperature is observed for lasers with a few picosecond pulse duration, whereas the temperature rise of acoustic and phonon temperatures is relatively small with decreasing laser pulse widths. A slight lagging behavior is observed due to the differences in relaxation times and heat capacities between two different phonons. Moreover, the laser fluence has a significant effect on the decaying rate of the Auger recombination.

Key Words: Ultra-Short Pulse, Micro-Scale Heat Transfer, Carrier Temperature, Optical Phonon, Acoustic Phonon, Nonequilibrium, Auger Heating

Nomenclature

C : Heat capacity per unit volume ($\text{J}/\text{m}^3 \cdot \text{K}$)	t : Time (s)
E_g : Band gap (eV)	t_p : Pulse duration time (full-width at half maximum) (s)
\mathfrak{S}_j : Fermi-Dirac integral of order j	T : Temperature (K)
h : Planck constant ($=6.6262 \times 10^{-34}$) ($\text{J} \cdot \text{s}$)	U : Internal energy (J/m^3)
I : Laser intensity (W/m^2)	y : Spatial coordinate (m)
J : Laser fluence (mJ/cm^2)	α_1 : One photon band-to-band absorption coefficient ($1/\text{m}$)
k_B : Boltzmann constant ($=1.38066 \times 10^{-23}$) (J/K)	δ : The impact ionization rate ($1/\text{s}$)
L : Thickness of a silicon film (m)	γ : Auger recombination coefficient (m^6/s)
N_C : Electron-hole pair (carrier) number density ($1/\text{m}^3$)	κ : Thermal conductivity ($\text{W}/\text{m} \cdot \text{K}$)
R : Reflectivity	λ : Wavelength (m)
	η : Reduced Fermi level
	ν : Photon frequency ($1/\text{s}$)
	τ_{C-O} : Energy relaxation time between carriers and LO phonons (s)
	τ_{C-A} : Energy relaxation time between carriers and acoustic phonons (s)
	τ_{O-A} : Energy relaxation time between LO phonons and acoustic phonons (s)

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Subscripts

- A* : Acoustic phonons
C : Carriers
O : Longitudinal optical (LO) phonons

1. Introduction

Recently, nonequilibrium energy transport during fast laser heating of materials has become a very important and challenging research subject. The advent of femtosecond pulse lasers made it possible to control the location and depth of heating precisely in fabricating microstructures, and it required a better understanding of radiation heating mechanisms from the microscopic viewpoint. Unlike metal substrates, energy transport in semiconductors depends on hot free electrons and holes. Figure 1 depicts the mutual interactions among photons, carriers (electron-hole pairs), and two phonons. Once laser energy deposits into materials, electron-hole pairs as energy carriers absorb photon energies of femto- to-picosecond pulse lasers which range from 1~5 eV. This range corresponds to a temperature level of about 10^4 K using $k_B T$ as the thermal energy of the electrons. Energy exchange takes place from hot carriers to phonons during the finite relaxation time which is typically in the range of 0.1 to 0.5 ps for silicon (Tien et al., 1998). When the laser pulse duration time is in the order of or shorter than this relaxation time, a substantial nonequilibrium occurs in semiconductors during laser irradiation under the condition when hot energetic carriers are not able to transfer their excess energy to the lattice efficiently. Since silicon has two atoms per unit cell, there are two different modes such as optical mode and acoustic mode. Since optical phonon energies are much higher than those of acoustic phonons, longitudinal optical (LO) phonons mostly encounter a very hot carrier reservoir in the range of $10^3 \sim 10^4$ K. The way for the energy carriers to lose their energy is to emit LO phonons since their wave vectors span the entire Brillouin zone at the same energy. The LO phonons possess negligible group velocity and thus do not contribute to

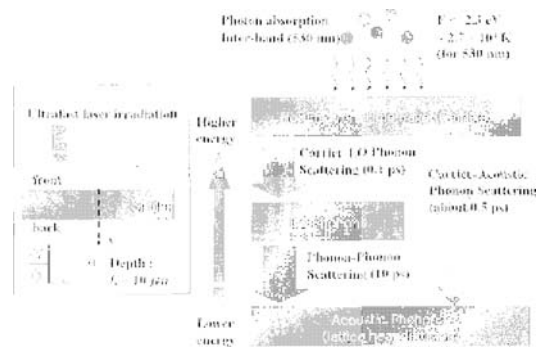


Fig. 1 Schematics for computational domain and mutual interactions among photons, electrons, LO phonons, and acoustic phonons

heat diffusion significantly. Eventually, LO phonons transfer their energies to acoustic phonons, which are responsible for lattice heat conduction.

Some of important parameters related to carriers and phonons, which are closely connected one another during rapid or slow heating process by the ultra-short pulse lasers, are extremely difficult to be directly measured by an experimental method because time and length scales are very small. The computational modeling offers a promising alternative to obtain detailed information on microscale heat transfer characteristics. From the particle point of view, however, even the numerical solutions are very difficult to be obtained because the Boltzmann transport equation (BTE) in six dimensions must be solved for electrons in each valley, optical phonons, and acoustic phonons. For avoiding this complexity and getting reasonable solutions physically, many researches have resorted mainly to hydrodynamic equations to model electron and phonon transport in practical engineering use. Qui and Tien (1994) 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. van Driel (1987) reported the kinetics of high-density plasmas generated in silicon by picoseconds laser pulse, found that the carrier temperature exhibited two peaks as a function of time due to laser heating as well as

Auger heating, and explained the interactions among the carrier number density, and carrier and lattice temperatures. These works mentioned above did not express interactions between LO phonons and acoustic phonons and most of investigators explained energy transport in radiative heating by ultrafast laser pulses by using only two temperatures for carriers and lattices. This two-temperature approach is based on the assumption that the lattice is a single thermodynamic system (Tien et al., 1998). This assumption is not valid generally because nonequilibrium energy transport process between two phonons exists clearly during very short but finite time scale. Tien et al. (1998) introduced an efficient way to represent the primary path of energy transport by first scattering between carriers and LO phonons and then LO phonons to the acoustic phonons. Their model can be hereafter referred to as the three-temperature model, which has been already used in studying thermal nonequilibrium in sub-micron silicon MOSFETs and GaAs MESFETs (Majumdar et al., 1995a, 1995b). To date (to the authors' knowledge), however, the use of three temperatures for ultrafast pulse laser heating problem has not been published in open literature. The ultimate goal of this study is thus posed to estimate time and spatial temperature distributions of carriers, LO phonons, and acoustic phonons to investigate their in-situ interactions and transports in solids during laser irradiation with subpicosecond pulses in silicon microstructures. The role of recombination process in the relaxation of carriers and phonons is also emphasized. For achieving this aim, the present study uses the original three-temperature model of Tien et al. (1998) basically, but some modifications are made for the present problems. In particular, the influence of laser fluences and pulse widths on nonequilibrium heat transfer is further examined.

2. Governing Equations and Properties

A detailed knowledge of mutual interactions among the heat carriers e.g. photon, electron

(hole), and phonon is required for analyzing micro-scale heat transfer phenomena. As for the carrier temperature much higher than the acoustic and LO phonon temperatures owing to the ultra-short pulse laser heating, especially, a consistent theoretical model should be derived to be able to describe the nonequilibrium between carriers and two phonons. In the case that photons incident on semiconductor have energies greater than the band gap energy of material, the main heat carrier is an electron-hole pair, whereas it is the free electron for metals (van Driel, 1987; Fushinobu et al., 1996; Seeger, 1991). The carrier number density of electron-hole pairs, N_c , is determined from the following conservation equation :

$$\frac{\partial N_c}{\partial t} = \frac{\alpha_1 I}{h\nu} - \gamma N_c^3 + \delta(T_c) N_c \quad (1)$$

$$I = \frac{0.939 J (1-R)}{t_p} \exp\left(-\int_0^y \alpha_l dz\right) \exp\left(-\frac{2.773 t^2}{t_p^2}\right) \quad (2)$$

where t is the time, γ the Auger recombination rate, N_c the carrier number density, h the Planck constant, I the laser intensity as a function of time and space, ν the photon frequency, $\delta(T_c)$ the impact ionization rate, and α_l is one photon band-to-band absorption coefficient. In Eq. (2), t_p is the pulse duration time with full width and half maximum (FWHM), J the laser fluence per pulse, and R is the reflectivity. The temporal change of the carrier number density is governed by three terms on the right-hand side of Eq. (1). The first term represents the absorption source term that corresponds to direct transition that excites an electron to the conduction band and creates an electron-hole pair, and the second term means the loss of the carriers through Auger recombination process in which the free electrons are captured by ionized donors and lose their energy non-radiatively (Pierret, 1983). The final term in Eq. (1) is the carrier generation rate owing to impact ionization process. Since the size of the laser beam is larger than the laser penetration depth, the short-pulse laser heating of materials can be modeled as one-dimensional.

As indicated by Tien et al. (1998), in most of previous work the lattice has been assumed to be

a single thermodynamic system. Because the time scales for carrier-optical phonon (typically 100fs) and phonon-phonon (10 ps) interactions are different by two orders of magnitude, however, this assumption cannot be rigorously justified. The three-temperature way is thus adopted in the present study and it uses the following energy conservation equations for carriers, LO phonons, and acoustic phonons separately (Tien et al., 1998):

$$\frac{\partial U_C}{\partial t} = \frac{\partial}{\partial y} \left(\kappa_C \frac{\partial T_C}{\partial y} \right) - \frac{3N_C k_B}{2\tau_{C-O}} (T_C - T_O) - \frac{3N_C k_B}{2\tau_{C-A}} (T_C - T_A) + \alpha_1 I \quad (3)$$

$$\frac{\partial U_O}{\partial t} = \frac{3N_C k_B}{2} \left(\frac{T_C - T_O}{\tau_{C-O}} \right) - C_O \left(\frac{T_O - T_A}{\tau_{O-A}} \right) \quad (4)$$

$$\frac{\partial U_A}{\partial t} = \frac{\partial}{\partial y} \left(\kappa_A \frac{\partial T_A}{\partial y} \right) + \frac{3N_C k_B}{2} \left(\frac{T_C - T_A}{\tau_{C-A}} \right) + C_O \left(\frac{T_O - T_A}{\tau_{O-A}} \right) \quad (5)$$

where the subscripts *C*, *O*, and *A* mean carriers, LO phonons, and acoustic phonons, respectively. In addition, *U* is the internal energy, *y* the spatial coordinate, κ the thermal conductivity, k_B the Boltzmann constant, *T* the temperature, and α_1 is the absorption coefficient. Equation (3) is the carrier energy conservation equation, which involves heat conduction by carriers, energy loss to optical phonons that takes place at a time scale of τ_{C-O} , energy loss to acoustic phonons at time scale τ_{C-A} , and an only source for total energy in the carrier system due to photon absorption. It should be noted that the assumption of Fourier law is not really valid for short time scale studies, but this is an approximation that invokes closure in the present type of hydrodynamic equation. The energy conservation for the optical phonons is expressed in Eq. (4), where the two terms on the right side represent energy gain from carriers and energy loss to acoustic phonons during the relaxation time τ_{O-A} . The final equation is that for acoustic phonons, where again the Fourier law is used for heat flux. Note that acoustic phonons possess finite group velocity and participate in heat diffusion. It means that the lattice temperature can be taken to be the acoustic phonon

temperature because this is the mode responsible for diffusion. Since optical phonons have negligible group velocity and cannot contribute to lattice heat conduction, on the other hand, there is no heat diffusion term in the right-hand side of Eq. (4). The only role of optical phonons is to provide an efficient intermediate path for heat transfer from the energy source due to photon absorption to the energy sink (acoustic phonons). This energy cascade substantially depends on carrier-to-LO phonon and phonon-to-phonon relaxation times, as well as heat capacities of carriers, LO phonons, and acoustic phonons. The internal energy of carrier *U_C* is expressed by $N_C E_B + (3N_C k_B T_C / 2) [\mathfrak{F}_{3/2}(\eta_e) / \mathfrak{F}_{1/2}(\eta_e) + \mathfrak{F}_{3/2}(\eta_h) / \mathfrak{F}_{1/2}(\eta_h)]$ where the function \mathfrak{F}_j is the Fermi-Dirac integral of order *j*, in terms of the reduced Fermi level η (van Driel, 1987). It is obvious that \mathfrak{F}_j can be approximated by e^η when $\eta \leq -3$, indicating that silicon is nondegenerate (Pierret, 1983). In addition, internal energies for LO phonons and acoustic phonons are represented by $U_O = C_O T_O$ and $U_A = C_A T_A$, respectively.

The physical properties should be determined definitely for the computations. Properties of silicon used in the present calculation are listed in Table 1, taken from related references (Tien et al., 1998; Agassi, 1984; Meyer et al., 1980; Wood and Giles, 1981; Jellison and Modine, 1982; Dziewior and Schmid, 1977; Jellison and Modine, 1983; Kittel, 1986; Raman et al., 2003). In particular, the heat capacities of two different phonons should be determined in a different manner. All the LO phonons are assumed to possess only one frequency from the typical dispersion relation for crystal vibrations. Einstein's model is adopted to approximate the heat capacity for silicon (Tien et al., 1998; Kittel, 1986). Since the acoustic phonons unlike the optical phonons have the group velocity of a wavepacket as the slope of the dispersion relation, Einstein's model is no longer valid. Thus, the heat capacity of acoustic phonons can be calculated using the Debye model which assumes the motion of neighboring atoms to be highly correlated (Kittel, 1986). A curve fit of silicon heat capacity is seen in Table 1, in terms of the

Table 1 Physical properties of a silicon layer

Physical Property	Value	Reference
Carrier heat capacity [J/m ³ ·K]	$C_C=3N_Ck_B$	(Agassi, 1984)
Acoustic phonon heat capacity [J/m ³ ·K]	$C_A=2.066 \times 10^6 - 9.91 \times 10^4 (\theta_D/T_A)^{1.946}$ where $\theta_D \approx 645\text{K}$ for silicon	(Kittel, 1986)
LO phonon heat capacity [J/m ³ ·K]	$C_o=2.49 \times 10^6 N_o k_B \left(\frac{\theta_E}{T_o}\right)^2 \frac{\exp(\theta_E/T_o)}{[\exp(\theta_E/T_o) - 1]^2}$ where $\theta_E = \hbar v/k_B \approx 731\text{K}$ for silicon	(Kittel, 1986)
Carrier thermal conductivity [W/m·K]	$\kappa_C = -0.556 + 7.13 \times 10^{-3} T_C$	(Agassi, 1984)
Acoustic phonon thermal conductivity [W/m·K]	$\kappa_A = 1.585 \times 10^5 T_A^{-1.23}$	(Wood and Giles, 1981)
Energy relaxation time [s]: carrier to acoustic phonon	$\tau_{C-A} = \tau_0 [1 + (N_C/N_{C,cr})^2]$ where $\tau_0 = 0.5 \times 10^{-12}$ and $N_{C,cr} = 2 \times 10^{27}$ (silicon)	(Agassi, 1984)
Energy relaxation time [s]: carrier to LO phonon	$\tau_{C-o} = 0.1$ ps	(Tien et al., 1998 ; Raman et al., 2003)
Energy relaxation time [s]: LD phonon to acoustic phonon	$\tau_{o-A} = 10$ ps	(Tien et al., 1998 ; Raman et al., 2003)
Absorption coefficient [1/m]	$\alpha_1 = 5.02 \times 10^5 \exp(-T_A/430)$, for $\lambda = 530$ nm	(Jellison and Modine, 1982)
Auger recombination coefficient, [m ⁶ /s]	$\gamma = 3.8 \times 10^{-43}$	(Dziewior and Schmid, 1977)
Reflectivity	$R = 0.37 + 5 \times 10^{-5} (T_A - 300)$ for $\lambda = 530$ nm	(Jellison and Modine, 1983)
Band gap [eV]	$E_g = 1.167 - 0.0258 [T_A/300] - 0.0198 [T_A/300]^2$	(Meyer et al., 1980)

Debye temperature θ_D and the acoustic temperature where $\theta_D = \hbar v_D/k_B \approx 645\text{K}$ for silicon (Kittel, 1986). Figure 2 represents the heat capacities of acoustic phonon and LO phonon with respect to the temperatures and compares them with the Dulong-Petit law (Kittel, 1986). LO phonon and acoustic phonon heat capacities have several orders of magnitude larger than the specific heat of carriers. For instance, the carrier heat capacity is approximately $10^{-5} \text{J/m}^3\text{-K}$ at 300K (Pierret, 1983), whereas the LO phonon and acoustic phonon specific heats are about $1.94 \times 10^6 \text{J/m}^3\text{-K}$ and $2.04 \times 10^6 \text{J/m}^3\text{-K}$ at 300K, respectively. This substantial difference becomes one of important factors, giving rise to the nonequilibrium phenomenon as discussed later. Meanwhile, for $\lambda = 530$ nm in the present study, two-photon and free carrier absorption can be neglected because single-photon inter-band absorption is very strong (van Driel, 1987). Furthermore, it is im-

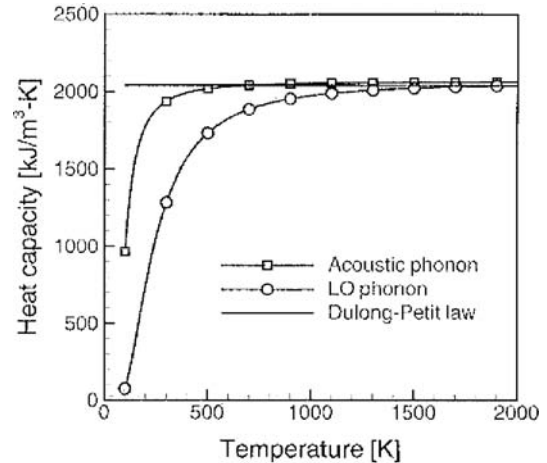


Fig. 2 The temperature functional behaviors of acoustic and LO phonon specific heats compared to the Dulong-Petit law

portant to determine the relaxation times due to scattering because the time scales of carrier-

phonon and LO phonon-acoustic phonons are quite different, giving rise to interesting dynamics. In silicon, the optical phonon energy is about 64 meV and the carrier-LO phonon relaxation time τ_{C-0} is in the range from 0.1 to 0.3 ps (Tien et al., 1998; Raman et al., 2003). During scattering of LO phonons and acoustic phonons, a characteristic time scale of τ_{0-A} is about 10 ps in silicon (Ferry, 1991) and the relaxation time of carriers and acoustic phonons can be given by the reference (Raman et al., 2003).

3. Computational Details

One-dimensional transient simulations are conducted using the finite difference methods to discretize the set of governing equations (Eqs. (1) and (3)~(5)). The initial time is set to $t_{init} = -5t_p$ for all cases. Initially, the carrier and the lattice temperatures are maintained at 300K, and the number density is 10^{18} m^{-3} (Pierret, 1983). As seen in Fig. 1, the von Neumann boundary conditions using the zero gradient at $y=0$ and $y=L$ are used in this work for temperatures of carrier and two phonons on the basis of the assumption that during the short period of laser heating, heat losses from the front and back surfaces of the silicon film may be negligible (Qiu and Tien, 1994). The final solutions are obtained when the relative deviation of each temperature is less than 10^{-4} and the residuals from energy equations are less than 10^{-9} likewise.

To investigate nonequilibrium energy transport characteristics on a silicon film irradiated by ultra-short pulse lasers, this article examines the temporal surface temperature distributions of carrier and two phonons (acoustic and LO) for three different laser pulse durations ($t_p=10.0, 50.0, 200.0$ ps) as well as two fluences of 50 and 150 mJ/cm^2 . For 530 nm radiation, all the simulations are performed for the case when $L=10 \mu\text{m}$. We take Gaussian pulses of various widths and the time step in numerical simulation must be taken carefully to capture the carrier-LO phonon scattering time scale of 0.1 ps. The effects of the time step and the mesh size on the final solutions are examined. As a result, the time step of 10 fs is

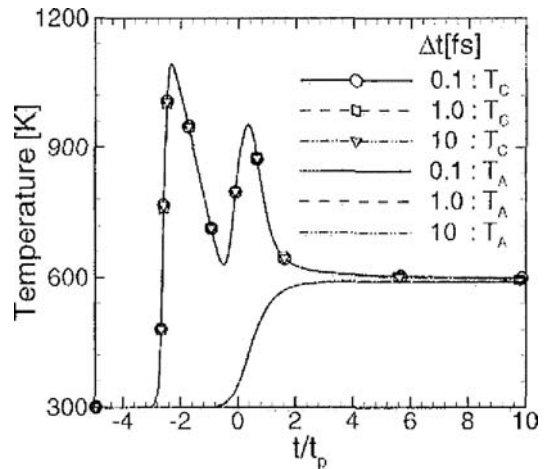


Fig. 3 Effect of the time step on the carrier and acoustic phonon temperatures for $J=150 \text{ mJ}/\text{cm}^2$ and $t_p=10$ ps

evaluated appropriate as seen in Fig. 3 and the mesh size used in all calculations is taken 20 nm through grid-independent tests.

4. Discussion

Figure 4 illustrates the time evolution of carrier, LO phonon, and acoustic phonon temperatures, and carrier number density for two different fluences when $\lambda=530$ nm and $t_p=10$ ps. A drastic increase in carrier temperature is observed for pulse lasers of a few picosecond duration, whereas the temperature rise of acoustic and LO phonons is relatively small. This significant non-equilibrium phenomenon is caused mainly by the difference between energy relaxation times and laser pulse durations. In particular, it is interesting to note an existence of two-peak structure in the carrier temperature because both the laser pulse and rapid Auger recombination heat the plasma and dominate as plasma heat sources at different times during the pulse, as was mentioned by Lee et al. (2003) and van Driel (1987). It indirectly suggests that thermal non-equilibrium state can be controlled by laser fluence as well as pulse duration time. The carrier temperature again rises near $t=0$, at which the number density increases and Auger recombination converts carrier ionization energy into kinetic energy at a

sufficiently large rate to again cause the carrier temperature to increase. From Fig. 4(b), the carrier number density increases during laser irradiation and its peak is increased with increasing laser fluence. The Auger recombination effects will be important during irradiation as the laser fluence increases because this type of recombination becomes dominant at high carrier concentrations in silicon. Once the carrier number density begins to decrease, the carrier temperature begins falling but the nonequilibrium between carrier and phonon temperatures maintains for long times owing to on-going Auger recombination (Lee et al., 2003). The nonequilibrium becomes disappearing as time goes on. Consequently, all energies are in equilibrium state as seen in Fig. 4(a). The maximum carrier temperatures for both fluences are estimated about 1000K, which corresponds to about 86 meV which is much smaller than incident photon energy of about 2.3 eV for 530 nm, whereas the equilibrium temperatures are observed 390K and 600K for $J=50$ and 150 mJ/cm², respectively. At the early stage of laser exposure, the carrier energies increases considerably due to carrier heat capacity much smaller than those of two phonons. After the finite time period, they lose energy to the phonons through emission of LO phonons, and the temperature difference between carriers and LO phonons drives energy transport flow. From Fig. 4(a), the time when LO phonon temperature begins to increase is slightly faster than that when acoustic phonon does. This behavior of time lagging is not only because the specific heat of LO phonons is a bit smaller than that of acoustic phonons as depicted in Fig. 2, but because there is the finite relaxation time between two phonons. In addition, at very short time duration, the energy transport from carriers to LO phonons dominates the problem resulting in nonequilibrium, leading to the rapid increase in LO phonon temperatures. This feature would be highly dependent on the physical properties of materials. For example, in GaAs or other III-V materials, even stronger coupling to electron-hole pairs will exist due to polar interactions and it makes LO phonons emitted more efficiently (Tien et al.,

1998 ; Kittel, 1986). Since optical phonon energies are higher than those of acoustic phonons as observed in Fig. 4(a), optical phonon emission is a faster and more efficient way of energy transfer. Eventually, optical phonons scatter and emit acoustic phonons, which are responsible for lattice heat conduction.

In situ behaviors of three different temperatures and carrier number densities are presented in Fig. 5 over the dimensionless time. It turns out that the peak laser intensity for the laser fluence decreases with increasing pulse duration. It leads

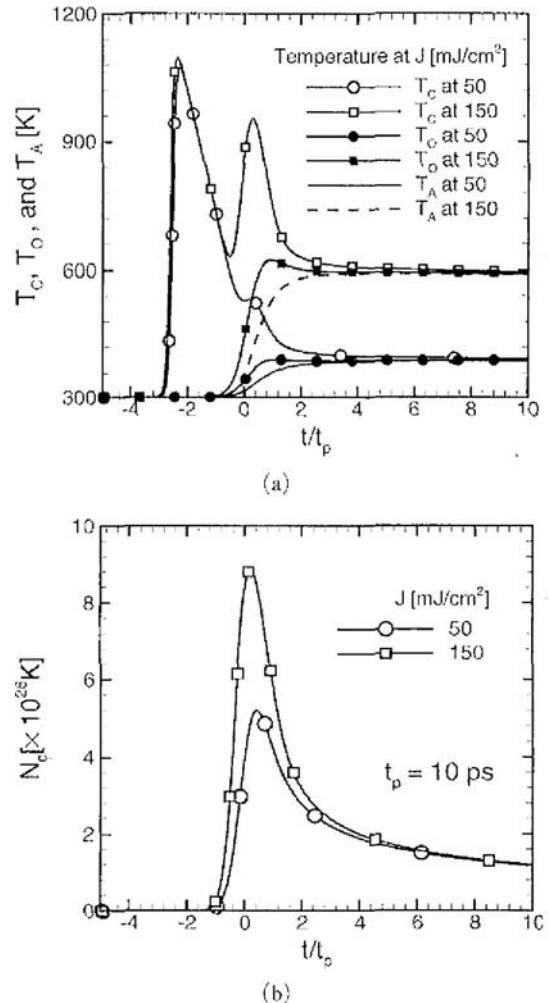


Fig. 4 Time evolutions of (a) carrier, LO phonon, acoustic phonon temperatures, and (b) carrier number densities for different fluences at $t_p=10$ ps

to the reduction in the peak value of carrier number density. Obviously, the extent of thermal nonequilibrium decreases as pulse duration increases, and carriers, optical phonons, and acoustic phonons are nearly in thermal equilibrium, although the initial increase in carrier temperatures is found at the early stage of laser irradiation. It is because the pulse durations are much larger than the relaxation times for carrier-phonon and phonon-phonon interactions. In the above discussion, it appears that the lattice temperature is hardly affected by the laser pulse, whereas it gradually increases with the laser flu-

ence. In addition, N_c increases with increasing laser fluence and its N_c^2 decaying rate is increased owing to Auger recombination.

Figures 6 and 7 illustrate the spatial temperature distributions of carriers, LO phonons, and acoustic phonons for different pulse durations, $t_p=10$ and 200 ps, respectively. All temperatures are calculated for silicon structures with a depth of 10 μm . For both cases, the maximum carrier diffusion depth is estimated about 3 μm when all temperatures are in equilibrium. In case when $t_p=10$ ps, Fig. 6 shows that at the early stage of irradiation, e.g., $t/t_p=-1.25$, very high nonequilibrium between carrier and phonon temperatures is present. It is natural that the nonequilibrium state for a short time should disappear eventually due to relaxation process. As expected, three temperatures become equilibrated as time goes.

Considering that the carriers transfer their energy to both LO phonons and acoustic phonons, it seems that much more energies are transferred from carriers to LO phonons because of faster relaxation time, compared to the carrier acoustic phonon scattering time. Note that LO phonon specific heat is smaller than approximately 1.5 times the acoustic phonon heat capacity at 300K. Owing to these facts, the LO phonon responds to the energies transferred from carriers faster than the acoustic phonons does. When the laser intensity peaks as seen in Fig. 6(b), the carrier temperature is about 860K at the front surface, whereas the LO and the acoustic temperatures are about 450K and 360K, respectively. Considering that the acoustic mode mostly contributes to the lattice heat conduction, the appearance of very high nonequilibrium means that the heat diffusion would be negligible during the laser-matter interaction and rapid energy deposition in carriers makes it feasible to recover stiction-failed microstructures using ultrashort pulse laser irradiation as were suggested by some researchers (Majumdar et al., 1995b; Lee et al., 2003; Tien et al., 1996).

Another important thing to note is that the lattice should not be regarded as a single thermodynamic system, widely used for many research-

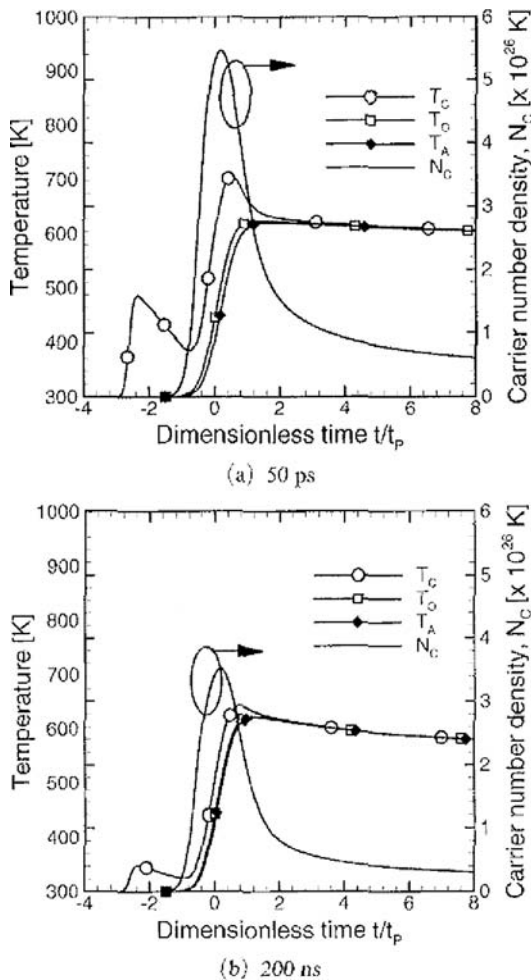


Fig. 5 In situ behaviors of carrier, LO phonon, acoustic phonon temperatures, and carrier number densities for 150 mJ/cm^2 at different pulse durations

chers for laser heating problems by very short pulses, where LO phonons and acoustic phonons are implicitly in equilibrium. For laser heating problems with subpicosecond pulse widths, more rigorous approach such as the three-temperature model used in the present study should be considered. Contrary to this, in the case when $t_p = 200$ ps, all temperatures as seen in Fig. 7 are nearly in equilibrium for a total duration of laser irradiation, because of pulse duration much larger than relaxation times. In this case, the thermal

equilibrium between two phonons would be a reasonable assumption for laser heating problems. As a matter of fact, a basic understanding of microscale energy transport from the above discussion is necessary to control the length of the nonequilibrium period, and it would be useful in applications in a variety of engineering fields where the nonequilibrium process between carriers and lattices is very important such as in microfabrication, laser heating, and stiction problems.

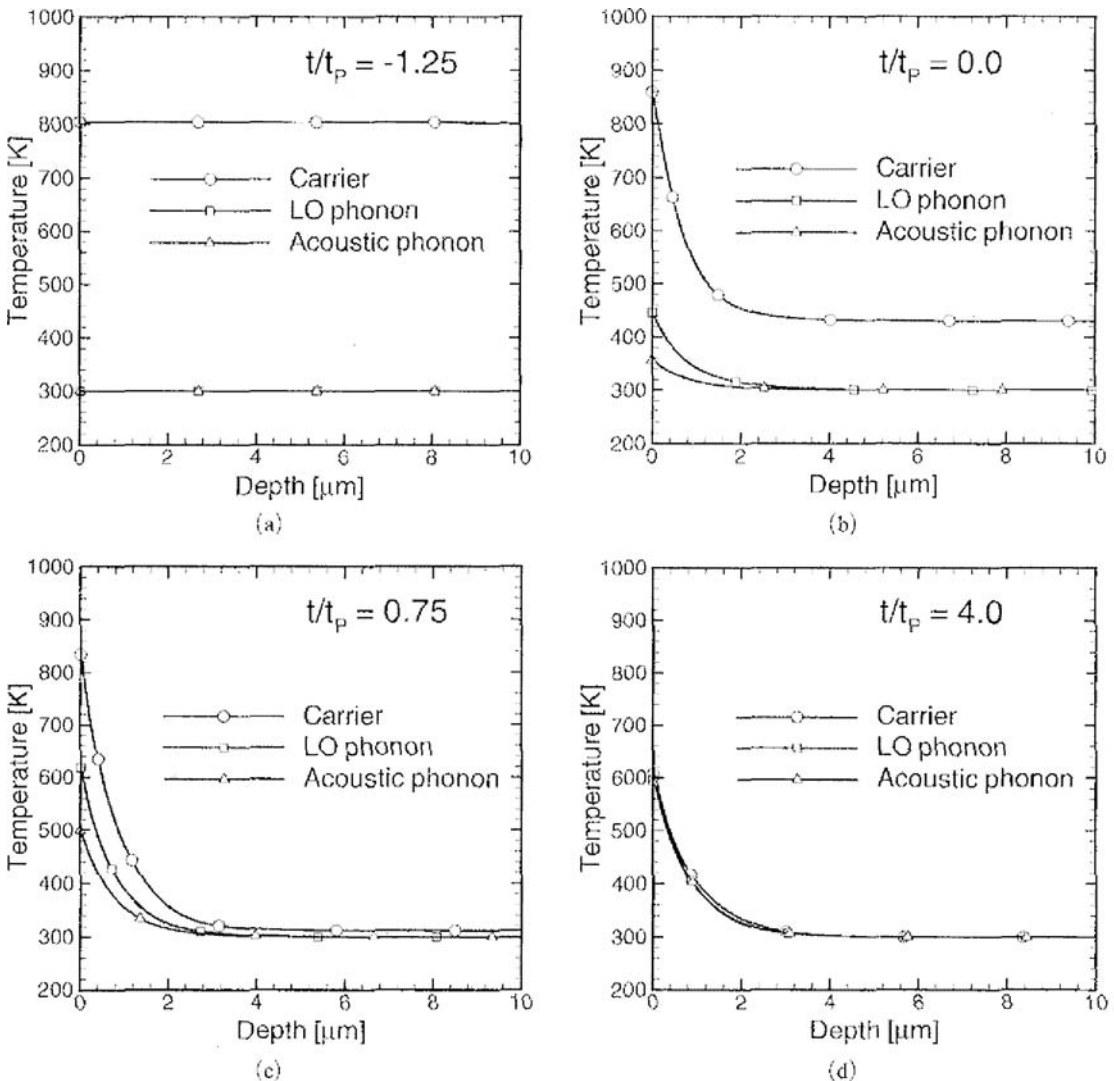


Fig. 6 Spatial temperature distributions of carriers, LO phonons, and acoustic phonons for 150 mJ/cm^2 and $t_p = 10 \text{ ps}$ at different time locations

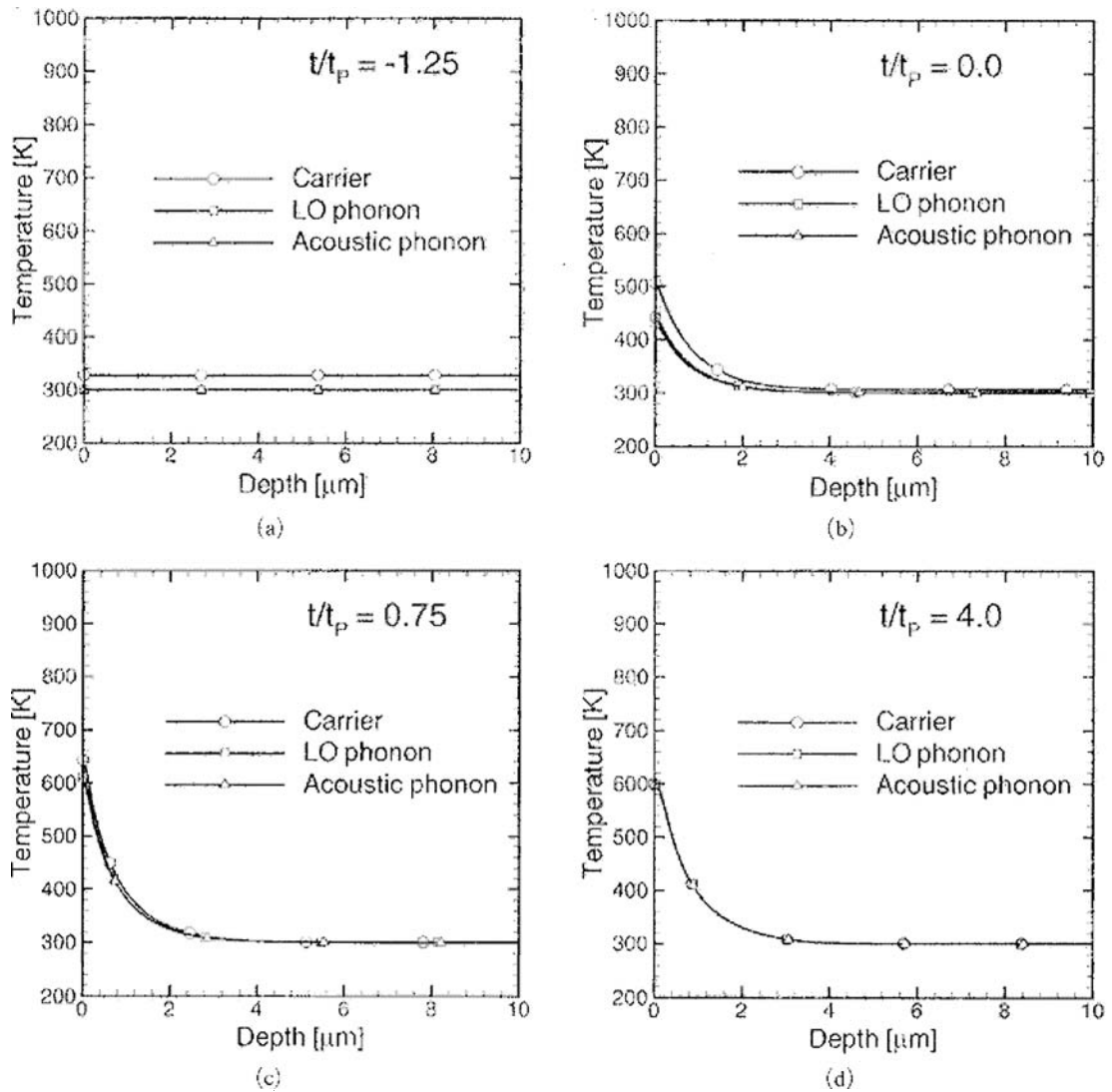


Fig. 7 Spatial temperature distributions of carriers, LO phonons, and acoustic phonons for 150 mJ/cm² and $t_p = 200$ ps at different time locations

5. Conclusions

The present article is devoted to provide the fundamental understandings of micro-scale heat transfer characteristics of a silicon film irradiated by ultra-short pulse laser. One-dimensional and transient analysis is extensively conducted by the three-temperature approach considering mutual interactions among carriers, LO phonons, and acoustic phonons. The influence of laser fluence and pulse duration time on heat transfer charac-

teristics are investigated and the following conclusions are drawn.

(1) At first, it is interesting to note that for ultrafast pulse laser heating, the assumption that a single thermodynamic system for LO phonons and acoustic phonons become no longer valid. The present study confirms that there are some difference and slight lagging behavior between LO and acoustic phonons. This is not only because the specific heats of two phonons are different, but also because the relaxation time of

carrier-LO phonon is smaller than that of LO phonon-acoustic phonon. However, for longer duration of laser pulse, thermally equilibrium assumption between two phonons is perhaps reasonable. It is also observed that the energy transport between carriers and LO-phonons dominates at very short time duration, leading to rapid increase in LO phonon temperatures.

(2) The maximum carrier temperature is estimated about 1000K, whereas the equilibrium temperature is about 600K for 150 mJ/cm^2 at $t_p = 10 \text{ ps}$. The scale difference between energy relaxation and laser pulse duration times gives rise to this thermal nonequilibrium state that can be controlled by laser fluence as well as pulse duration time. This confirms the feasibility of moisture removal problem, which is often confronted in microstructure fabrication.

(3) A two-peak structure of carrier temperature is observed to take place owing to Auger recombination as well as scale difference between pulse width and relaxation times. In addition, it is found that the extent of thermal nonequilibrium decreases as pulse duration decreases, and the carrier number density increases and its N^3 decaying rate is increased owing to Auger recombination with increasing laser fluence.

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