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A generalized heat conduction solution for ultrafast laser heating in metallic films

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ABSTRACT

A generalized analytical solution for the electron and lattice temperature profiles in a metallic film exposed to an ultrafast laser source is obtained using the superposition and Fourier methods in conjunction with solution structure theorems. The generalized temperature profile in algebraic form is applicable for the solution of three thermal models, namely, phonon–electron two-temperature interaction model, electron kinetic theory model, and the improved electron kinetic theory model. By selecting the appropriate coefficients as appear in the original governing partial differential equation of a particular model, temperature profiles for both the electron and lattice can readily be obtained. A comparison of the aforementioned models in graphical form is made. Results from the phonon–electron two-temperature interaction model agree well with the improved electron kinetic theory model for electron and lattice temperatures. However, due to the omission of the time rate change of heat diffusion and laser source, temperature predictions from the electron kinetic theory model are slightly higher than temperatures from the other two models; particularly, the effect is more profound at the location of the energy incident surface. Otherwise all three models compare extremely well for the lattice site temperatures.

1. Introduction

Given the prevalence of ultrafast laser processing in the manufacturing industry involving fast laser heating of solids, an ability to model the energy transport process accurately in micro/nanoscale is important. The heat transfer mechanism and thermal lagging behavior in metallic materials have been a subject of theoretical investigation with great interest for the past several decades. Many studies have focused on nonequilibrium temperatures between electron and lattice in ultrasfast pulsed laser applications. The energy transport phenomenon within the substructure for such applications takes finite time to process and therefore it is given the term "lagging behavior" to describe the mechanism. Based on quantum theory, the energy state of a metal lattice can be viewed as quanta or phonons. Thermal energy transport involves two stages when a metallic surface is subjected to laser radiation heating. First, photons from the laser warm up the electron gas while the metal lattice temperature remains unchanged. Through inelastic phonon–electron scattering and interactions, the incident radiation energy absorbed by the metal lattice diffuses spatially and raises the lattice temperature. This phenomenon ranges from a delay of several seconds to nanoseconds, picoseconds or even femtoseconds. Therefore the interstructural interaction takes place at a finite time rather than instantaneous time and such action does not follow the Fourier theory. A detailed explanation of the process is available in the textbook by Tzou [1].

Techniques for modeling the heating mechanism in metals first appeared in the late 1950s and new analytical techniques are still being developed. Heat transport in metals can be modeled based on the conventional parabolic one-step Fourier diffusion theory [2] or by the hyperbolic one-step model [2]. Since the energy transport mechanism is conduction through electron–phonon interaction within the microstructure, these two models neglect the microenergy transfer when the heating process is relatively fast and consequently, their applicability is invalid. To include these effects, newer models are developed that are more complex, and can be categorized as either parabolic or hyperbolic two-step models.

The energy transport phenomenon was first investigated theoretically by Kaganov et al. [3], followed by Anisimov et al. [4] with a phonon–electron two-temperature interaction model to describe both phonon and electron temperatures during the thermal interaction process. The nonequilibrium temperature difference between electrons and phonons in this phenomenon was later confirmed by Fujimoto et al. [5], Brorson et al. [6], Eesley [7], and Qiu and Tien [8,9]. In the phonon–electron two-temperature interaction

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Nomenclature

$\mathcal{A}$	constant, Eq. (11)
$\mathcal{B}$	constant, Eq. (11)
$\mathcal{C}$	constant, Eq. (11)
C_e	electron heat capacity, J/m^3 K
C_l	lattice heat capacity, J/m^3 K
C_p	specific heat of lattice site, J/kg K
$C_1 \ldots C_{17}$	coefficients, Eqs. (23) and (24)
$\mathcal{D}$	constant, Eq. (11)
f	total energy in system, W/m^3
f_{ex}	fraction of excess energy site, J/kg K
$\mathcal{F}$	functional form for Sub-problem 1
G	electron phonon coupling factor, W/m^3 K
G_l	energy magnitude factor at the left boundary
G_r	energy magnitude factor at the right boundary
g	source term, W/m^3
g_l	energy strength at the left boundary, $G_l(1-R)J_o\mu$, W/m^3
g_r	energy strength at the right boundary, $G_r(1-R)J_o\mu$, W/m^3
J_o	laser fluence, W/m^2
k	thermal conductivity, W/m K
$\bar{k}$	extinction coefficient
L	film thickness, m
$\mathcal{M}$	constant, Eq. (12)
$\mathcal{N}$	constant, Eq. (12)
$\bar{n}$	refractive index
R	surface reflectivity
t	time, s
t_p	energy pulse time, s
T	temperature, K
T_o	initial temperature, K
T_1	temperature solution due to ψ function contribution, K
T_2	temperature solution due to φ function contribution, K
T_3	temperature solution due to total energy in system f function contribution, K
x	spatial coordinate, m

Greek symbols

β_n	eigenvalue, Eq. (19f)
γ_n	eigenvalue, Eq. (20a)
ζ	dummy variable for time
ϑ_n	eigenvalue, Eq. (19e)
λ	mean free path of electrons, m
λ_o	wavelength in vacuum, nm
λ_n	eigenvalue, Eq. (19d)
μ	absorption coefficient, m^{-1}
ξ	dummy variable for space
ρ	density, kg/m^3
τ_p	electron mean free time between electron–phonon coupling, s
τ_s	electron–phonon characteristic time, C_e/G, s
φ	initial condition function, K
ψ	initial rate of temperature change function, K/s
ϖ_n	constant, Eq. (20b)

Subscripts

e	electron
l	lattice
n	series solution index

model, the thermal behavior of a metal is characterized with two energy balances between electrons and phonons. These two systems are coupled via the electron–phonon coupling factor. By taking the electron kinetic theory approach for the laser short-pulse heating process, Yilbas [10] advanced the phonon–electron two-temperature interaction model by developing the electron kinetic theory model. However, the model neglects the rate of change for diffusion as well as the energy source. With the inclusion of these two terms, an improved electron kinetic theory model was later formulated by Yilbas [11]. The primary focus of this paper will be concentrated on the solution of the electron and lattice site temperatures based on the three models mentioned above.

The phonon–electron two-temperature interaction model has been solved with the Crank–Nicholson scheme with a non-uniform grid system by Qiu and Tien [8,9]. Results were compared with the one-step [2] and two-step parabolic [4] and hyperbolic one-step [12] and two-step [9] theoretical models as well as experimental data [6] revealing that the parabolic two-step model [4] was able to predict the general trend of the temperature response but fails to predict the finite speed propagation phenomenon. This discrepancy was investigated by Tzou et al. [13]. The study divulged that although a wave term is present in the microscopic parabolic two-step model governing the metal lattice, the sharp wavefront was nonexistent as a result of the strong dispersion during the phonon–electron interaction process. Nevertheless, it was concluded that the two-step model is still a valid tool since it provides more valuable temperature information for the transient process especially for ultrafast heating applications.

Al-Mimr and Arpaci [14] introduced a simplified approach to study the thermal behavior of a thin metal film exposed to thermal pulses of picosecond duration with the parabolic two-step model. The thermal behavior of the metal film occurs in two separate stages. Energy transport in both stages is either dominated by the electron gas energy transmission to the solid lattice through electron–phonon coupling or by thermal diffusion. During the process, all other energy transport mechanisms become negligible. With such an approach, the coupling effect between the energy equation of both the solid lattice and electron gas is reduced. As a result, the reduced partial differential equations become simpler from a mathematical point of view. In a subsequent study, Al-Mimr and Masoud [15] employed a perturbation technique to decouple the electron gas and lattice energy as they appear in the two-step model when the temperature difference between them becomes sufficiently small. The resulting two uncoupled partial differential equation contain no mixed derivative terms enabling the study of nonequilibrium temperatures during laser heating of metal films with ease.

It is well known that the conventional Fourier heat conduction model is not applicable for the study of short-pulse heating of metals due to the infinite speed assumption associated with the theory. Yilbas [10] initiated an electron kinetic theory approach to improve the temperature solution for short pulse heating applications. The temperature solution was obtained by using a finite-difference scheme and the results revealed that the parabolic one-equation model predicts excessive temperature rise at the surface subjected to thermal radiation exposure. The same approach was used for the study of picosecond laser pulse heating of metals [10]. Identical temperature results were obtained between the two-step temperature model and the electron kinetic theory approach [16].

Analytical solution for the phonon–electron two-temperature interaction model has received a great deal of interest in the past. Yilbas et al. [17] obtained a numerical temperature solution of a gold film subjected to laser short pulse heating and used that temperature solution as the initial condition to the two-temperature governing equations of energy transport. The perturbation method