

Symmetries and approximate solution of energy transfer equations in short pulse laser heating

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Abstract

Energy transfer equations in laser heating are considered. Symmetries of the equations are calculated by Lie Group theory. Using the symmetries, the equations are transferred to an ordinary differential system. Equations are approximately solved by strained parameter method, a perturbation technique. A boundary value problem in which the laser beam transfers heat to the surface is treated. Closed form approximate solutions for electron and lattice site temperature rise are obtained for a solid layer heated at the surface with a time decaying intensity pulse. Analytical solutions are verified by numerical simulations.

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1. Introduction

Non-equilibrium energy transport occurs in metallic solids when high intensity heat fluxes are deposited on to substrate surface within a duration equal or less than the thermalization time of the substrate material. In this case, electron and lattice sub-systems separate thermally and the collisional process defines the energy transport between the sub-systems. Electrons receive energy from the heating source resulting in increasing electron excess energy. Moreover, electrons transfer some fraction of their excess energy to lattice site through electron-lattice site collisions. This results in lattice site energy increase; consequently, lattice site temperature increases gradually as the collisional process for energy transport from electron to lattice sub-systems continues. Since the electron and lattice sub-system separates thermally, modeling of the energy transport on the microscopic scale becomes necessary. The analytical solution for such a physical problem is fruitful, since it provides

a functional relationship between electron and lattice temperatures.

The energy transport equations modeling this phenomenon are treated analytically by considering the symmetries of the differential equations. The symmetries may be used to produce group-invariant (similarity) solutions. A partial differential system with 2 independent variables can be transformed to an ordinary differential system which would be easier to solve. Symmetries can be calculated using two major approaches: (1) Lie Group theory (2) Exterior differential form method. The theory is involved and relevant information can be found in the previous literature. For details of Lie Group theory, see [1–3] and for those of Exterior Differential Form method, see [4–6].

In this study, symmetries of the energy transport equations are calculated first. To the best of the authors' knowledge, this has not been done before. Using a special symmetry, the partial differential system is transformed to an ordinary differential system. A physical small parameter appears when equations are cast into a non-dimensional form and a perturbation solution is possible in terms of this small parameter. Strained parameters method is used as the perturbation technique. The approximate solution is then applied to a specific boundary value problem.

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Nomenclature

a, b, c	finite Lie Group transformation parameters	T_0	reference temperature
d	inverse of mean free path of electrons ($= 1/\lambda$)	X	infinitesimal generator
f	infinite Lie Group transformation parameter	α	dimensionless thermal conductivity
k	thermal conductivity	λ	mean free path of electrons
k_1	exponential source decay parameter	λ_1	parameter related to m_0 and α through Eq. (21)
m	similarity parameter	ε	ratio of heat capacities
$m_{1,2}$	first and second terms of similarity parameter in the perturbation expansion	μ	similarity variable
t	dimensionless time	$\xi_{1,2}$	infinitesimals for independent variables
\bar{t}	dimensional time	$\eta_{1,2}$	infinitesimals for dependent variables
x	dimensionless lattice depth	θ_E	dimensionless electron temperature
\bar{x}	dimensional lattice depth	θ_L	dimensionless lattice site temperature
C_E	electron heat capacity	$\theta_{L0,L1}$	first and second terms of dimensionless lattice site temperature in the perturbation expansion
C_L	lattice heat capacity	θ_0	dimensionless limit temperature after a long time
G	electron–phonon coupling factor	I_0	dimensionless source amplitude
T_E	electron temperature	\bar{I}_0	dimensional source amplitude
T_L	lattice site temperature		

An infinite (considerably thick) depth material is heated from the surface by a time decaying heat source. The perturbation solution obtained is contrasted with a direct numerical solution of the partial differential system. In the numerical solution, a finite difference scheme is employed. Electron and Lattice site temperatures are plotted with varying spatial variable and time. Numerical and analytical results are in good agreement.

Some of the relevant papers on the topic are mentioned as follows: Yılbaş [7] introduced the electron kinetic theory approach to model the non-equilibrium heating situations. Yılbaş and Şahin [8] obtained a closed form solution for lattice site temperature rise for step input laser pulse intensity. The non-local heat transport due to steep temperature gradients was studied by Luciani et al. [9]. They developed a formula for the non-local thermal heat flux. The electron–phonon relaxation in copper was measured by Elsayed-Ali et al. [10]. They observed the non-equilibrium electron and lattice temperatures in copper during high intensity short-duration of heating. The ultra fast heat transport dynamics in gold films was investigated by Brorson et al. [11]. They showed that heat transit time scales linearly varied with the work-piece thickness. Thermal relaxation of electrons in metals was studied by Allen [12]. He developed a simplified equation for the thermal relaxation rate. Laser picosecond heating of thin films was examined by Al-Nimr and Arpacı [13]. They developed the energy transport equations and introduced the criteria for the applicability of the decoupling of the energy equations. They indicated that the formula introduced agreed well with the numerical results obtained from Fokker–Planck equation. Electron temperature measurement was carried out by Wang et al. [14]. They showed that room temperature thermal properties were modified considerably at elevated electron temperatures. The analytical solution of a unified heat conduction equation was presented by Lin et al. [15]. Their solution was based on the method of separation. The wave diffusion and parallel non-equilibrium heat

conduction was examined by Honner and Kunes [16]. They developed the key parameters to classify the heating situation. Chen [17] investigated ballistic-diffusive heat conduction equations. He suggested that the proposed formulation was a better approximation than the Fourier and the Cattonea equations for heat conduction. Finally, Yılbaş et al. [18] solved approximately the energy transport equations for the cooling period of an initially heated thin film by perturbation techniques.

Although the model considered in this study is the same with the one treated in [18], the analysis differs in a number of ways: In that study, a finite depth was taken, but here semi-infinite substrate material is considered. The solution [18] corresponds to a cooling of an initially heated material with isolated boundary conditions whereas time decaying heat source is applied to the surface in this study. Compared to the purely perturbative solution in [18], a similarity type solution combined with perturbation analysis is presented here. The analytical solution is also verified with direct numerical simulations.

2. Mathematical model

The energy transport equation for electron and lattice subsystems without source term can be written as [18]:

$$C_E \frac{\partial T_E}{\partial \bar{t}} = k \frac{\partial^2 T_E}{\partial \bar{x}^2} - G(T_E - T_L) \quad (1)$$

$$C_L \frac{\partial T_L}{\partial \bar{t}} = G(T_E - T_L) \quad (2)$$

where T_E and T_L are the electron and lattice site temperatures respectively. C_E is the electron heat capacity, C_L is the lattice heat capacity, G is the electron–phonon coupling factor and k is the thermal conductivity. \bar{x} is the dimensional lattice depth and \bar{t} is the dimensional time. If the dimensionless quantities are defined as

$$\theta_{E,L} = \frac{T_{E,L}}{T_0}, \quad x = \bar{x}d, \quad t = \frac{\bar{t}}{C_E/G} \quad (3)$$

Eqs. (1) and (2) reduce to the following form

$$\frac{\partial \theta_E}{\partial t} = \alpha \frac{\partial^2 \theta_E}{\partial x^2} - (\theta_E - \theta_L) \quad (4)$$

$$\frac{\partial \theta_L}{\partial t} = \varepsilon (\theta_E - \theta_L) \quad (5)$$

where

$$\alpha = \frac{kd^2}{G}, \quad \varepsilon = \frac{C_E}{C_L} \quad (6)$$

In the above formulation, $d = 1/\lambda$ and λ is the mean free path of electrons. In a variety of applications, dimensionless thermal conductivity α is of order 1 and the ratio of heat capacities ε is small compared to order 1 terms. Therefore, as will be shown later, a perturbation type of solution in terms of the small parameter ε is possible. Before applying perturbations, in the next section, the symmetries of the model will be calculated first. This will enable us to transfer the model from a partial differential system to an ordinary differential system. A perturbation solution of the ordinary differential system will follow then.

3. Symmetries and a similarity transformation

Lie Group theory [1–3] will be applied to Eqs. (4) and (5). The infinitesimal generator for the problem can be written as

$$X = \xi_1 \frac{\partial}{\partial x} + \xi_2 \frac{\partial}{\partial t} + \eta_1 \frac{\partial}{\partial \theta_E} + \eta_2 \frac{\partial}{\partial \theta_L} \quad (7)$$

In the standard procedure, Eqs. (4) and (5) are re-written using higher order variables as follows

$$u_1^1 = \alpha u_{11}^1 - (u^1 - u^2) + \beta S(x_1, x_2) \quad (8)$$

$$u_2^2 = \varepsilon (u^1 - u^2) \quad (9)$$

where new variables are defined for convenience

$$x_1 = x, \quad x_2 = t$$

$$u^1 = \theta_E, \quad u^2 = \theta_L, \quad u_{11}^1 = \frac{\partial \theta_E}{\partial x_2}$$

$$u_2^2 = \frac{\partial \theta_L}{\partial x_2}, \quad u_{11}^1 = \frac{\partial^2 \theta_E}{\partial x_1^2} \quad (10)$$

Generator (7) is prolonged to higher order variables

$$X = \xi_1 \frac{\partial}{\partial x_1} + \xi_2 \frac{\partial}{\partial x_2} + \eta^1 \frac{\partial}{\partial u_1} + \eta^2 \frac{\partial}{\partial u_2} + \eta_2^{(1)1} \frac{\partial}{\partial u_1^1} + \eta_2^{(1)2} \frac{\partial}{\partial u_2^1} + \eta_{11}^{(2)1} \frac{\partial}{\partial u_{11}^1} \quad (11)$$

Applying the prolonged generator to Eqs. (8) and (9) yields the invariance conditions

$$\eta_2^{(1)1} = \alpha \eta_{11}^{(2)1} - (\eta^1 - \eta^2) + \beta \left(\xi_1 \frac{\partial S}{\partial x_1} + \xi_2 \frac{\partial S}{\partial x_2} \right) \quad (12)$$

$$\eta_2^{(1)2} = \varepsilon (\eta^1 - \eta^2) \quad (13)$$

$\eta_2^{(1)1}$, $\eta_2^{(1)2}$, $\eta_{11}^{(2)1}$ are to be expressed in terms of ξ_1 , ξ_2 , η_1 , η_2 using the standard recursion formulas [1–3]. The invariance conditions can be treated as polynomials in terms of defined

higher order variables. Hence, equating the coefficients of those polynomials on both sides yields a set of over-determined partial differential system. Invariance condition (13) after separation yields

$$\begin{aligned} \frac{\partial \eta^2}{\partial x_2} + \varepsilon (u^1 - u^2) \left(\frac{\partial \eta^2}{\partial u^2} - \frac{\partial \xi_2}{\partial x_2} \right) - \varepsilon^2 (u^1 - u^2)^2 \frac{\partial \xi_2}{\partial u^2} \\ = \varepsilon (\eta^1 - \eta^2) \end{aligned} \quad (14)$$

$$\frac{\partial \eta^2}{\partial u^1} - \varepsilon (u^1 - u^2) \frac{\partial \xi_2}{\partial u^1} = 0 \quad (15)$$

$$\frac{\partial \xi_1}{\partial x_2} + \varepsilon (u^1 - u^2) \frac{\partial \xi_1}{\partial u^2} = 0 \quad (16)$$

$$\frac{\partial \xi_1}{\partial u^1} = 0 \quad (17)$$

Invariance condition (12) yields

$$\begin{aligned} \frac{\partial \eta^1}{\partial x_2} + \varepsilon (u^1 - u^2) \frac{\partial \eta^1}{\partial u^2} \\ = \alpha \left\{ \frac{\partial^2 \eta_1}{\partial x_1^2} + \frac{1}{\alpha} [u^1 - u^2 - \beta S] \left(\frac{\partial \eta^1}{\partial u^1} - 2 \frac{\partial \xi_1}{\partial x_1} \right) \right\} \\ - (\eta^1 - \eta^2) + \beta \left(\xi_1 \frac{\partial S}{\partial x_1} + \xi_2 \frac{\partial S}{\partial x_2} \right) \end{aligned} \quad (18)$$

$$\begin{aligned} \frac{\partial \eta^1}{\partial u^1} - \frac{\partial \xi_2}{\partial x_2} - \varepsilon (u^1 - u^2) \frac{\partial \xi_2}{\partial u^2} \\ = \alpha \left\{ -\frac{\partial^2 \xi_2}{\partial x_1^2} + \frac{1}{\alpha} \left(\frac{\partial \eta^1}{\partial u^1} - 2 \frac{\partial \xi_1}{\partial x_1} \right) \right. \\ \left. - \frac{1}{\alpha} [u^1 - u^2 - \beta S] \frac{\partial \xi_2}{\partial u^1} \right\} \end{aligned} \quad (19)$$

$$\begin{aligned} -\frac{\partial \xi_1}{\partial x_2} - \varepsilon (u^1 - u^2) \frac{\partial \xi_1}{\partial u^2} \\ = \alpha \left\{ 2 \frac{\partial^2 \eta^1}{\partial u^1 \partial x_1} - \frac{\partial^2 \xi_1}{\partial x_1^2} - \frac{3}{\alpha} [u^1 - u^2 - \beta S] \frac{\partial \xi_1}{\partial u^1} \right\} \end{aligned} \quad (20)$$

$$\frac{\partial \xi_1}{\partial u^1} = \alpha \left\{ 2 \frac{\partial^2 \xi_2}{\partial u^1 \partial x_1} + \frac{3}{\alpha} \frac{\partial \xi_1}{\partial u^1} \right\} \quad (21)$$

$$\frac{\partial^2 \eta^1}{\partial u^2 \partial x_1} - \frac{1}{\alpha} [u^1 - u^2 - \beta S] \frac{\partial \xi_1}{\partial u^2} = 0 \quad (22)$$

$$\frac{\partial^2 \eta^1}{\partial u^1^2} - 2 \frac{\partial^2 \xi_1}{\partial u^1 \partial x_1} = 0 \quad (23)$$

$$\frac{\partial^2 \eta^1}{\partial u^1 \partial u^2} - \frac{\partial^2 \xi_1}{\partial u^2 \partial x_1} = 0 \quad (24)$$

$$\frac{\partial^2 \xi_2}{\partial x_1 \partial u^2} + \frac{1}{\alpha} \frac{\partial \xi_1}{\partial u^2} = 0 \quad (25)$$

$$\frac{\partial^2 \xi_1}{\partial u^1^2} = 0 \quad (26)$$

$$\frac{\partial^2 \xi_1}{\partial u^1 \partial u^2} = 0 \quad (27)$$

$$\frac{\partial^2 \xi_2}{\partial u^1^2} = 0 \quad (28)$$

$$\frac{\partial^2 \xi_2}{\partial u^1 \partial u^2} = 0 \quad (29)$$

$$\frac{\partial^2 \eta^1}{\partial u^{2^2}} = 0 \quad (30)$$

$$\frac{\partial^2 \xi_1}{\partial u^{2^2}} = 0 \quad (31)$$

$$\frac{\partial^2 \xi_2}{\partial u^{2^2}} = 0 \quad (32)$$

$$\frac{\partial \xi_2}{\partial x_1} = 0 \quad (33)$$

$$\frac{\partial \xi_2}{\partial u^1} = 0 \quad (34)$$

$$\frac{\partial \xi_2}{\partial u^2} = 0 \quad (35)$$

$$\frac{\partial \eta^1}{\partial u^2} = 0 \quad (36)$$

$$\frac{\partial \xi_1}{\partial u^2} = 0 \quad (37)$$

$$\frac{\partial \xi_2}{\partial u^2} = 0 \quad (38)$$

Partial differential system (14)–(38) is an over-determined system, which can be solved easily for the infinitesimals. Solving the system and returning back to the original variables yield

$$\xi_1 = a$$

$$\xi_2 = b$$

$$\eta_1 = c\theta_E + \frac{1}{\varepsilon} \frac{\partial f}{\partial t} + f(x, t)$$

$$\eta_2 = c\theta_L + f(x, t) \quad (39)$$

where the structure of $f(x, t)$ is determined by the below equation

$$\frac{\partial^2 f}{\partial t^2} + (\varepsilon + 1) \frac{\partial f}{\partial t} - \alpha \frac{\partial^3 f}{\partial x^2 \partial t} - \alpha \varepsilon \frac{\partial^2 f}{\partial x^2} = 0 \quad (40)$$

Parameters a , b and c represent finite Lie point symmetries whereas $f(x, t)$ is an infinite Lie point symmetry.

From the symmetries, a similarity solution can be constructed using the parameters a and b and selecting $c = 0$, $f(x, t) = 0$. The determining equations for this choice is

$$\frac{dx}{a} = \frac{dt}{b} = \frac{d\theta_E}{0} = \frac{d\theta_L}{0} \quad (41)$$

Solving the system, the similarity variable and functions are determined

$$\mu = x - mt, \quad \theta_E = \theta_E(\mu), \quad \theta_L = \theta_L(\mu) \quad (42)$$

where $m = a/b$. Substituting the variables into Eqs. (4) and (5) yields

$$-m\theta'_E = \alpha\theta''_E - (\theta_E - \theta_L) \quad (43)$$

$$-m\theta'_L = \varepsilon(\theta_E - \theta_L) \quad (44)$$

where prime denotes differentiation with respect to the similarity variable μ . Solving the last equation for θ_E

$$\theta_E = -\frac{m}{\varepsilon} \theta'_L + \theta_L \quad (45)$$

and inserting into Eq. (43) one has

$$\alpha\theta'''_L + \left(m - \varepsilon \frac{\alpha}{m}\right) \theta''_L - (1 + \varepsilon) \theta'_L = 0 \quad (46)$$

4. Perturbation solution

In a variety of applications, the ratio of heat capacities (i.e. parameter ε) is rather small, hence a perturbation type of solution is possible. Since the straightforward expansion breaks down due to secular terms, strained parameters method will be employed [19]. In accordance, the dependent variable as well as the similarity parameter m is expanded in a perturbation series

$$\theta_L = \theta_{L0} + \varepsilon\theta_{L1} + \dots \quad (47)$$

$$m = m_0 + \varepsilon m_1 + \dots \quad (48)$$

Inserting the expansions into Eq. (46) and separating at each order yields

$$O(1): \quad \alpha\theta'''_{L0} + m_0\theta''_{L0} - \theta'_{L0} = 0 \quad (49)$$

$$O(\varepsilon): \quad \alpha\theta'''_{L1} + m_0\theta''_{L1} - \theta'_{L1} \\ = -m_1\theta''_{L0} + \frac{\alpha}{m_0}\theta''_{L0} + \theta'_{L0} \quad (50)$$

The solution at order 1 is

$$\theta_{L0} = c_1 + c_2 e^{\lambda_1 \mu} + c_3 e^{\lambda_2 \mu} \quad (51)$$

where

$$\lambda_1 = \frac{-m_0 - \sqrt{m_0^2 + 4\alpha}}{2\alpha}, \quad \lambda_2 = \frac{-m_0 + \sqrt{m_0^2 + 4\alpha}}{2\alpha} \quad (52)$$

For decaying type of solutions, $c_3 = 0$ should be selected. Inserting this solution into the next order and eliminating secular terms yields

$$m_1 = \frac{\alpha}{m_0} - \frac{2\alpha}{m_0 + \sqrt{m_0^2 + 4\alpha}} \quad (53)$$

Returning back to the original variables, calculating θ_E from Eq. (45), the approximate solutions can be written as follows

$$\theta_L = c_1 + c_2 e^{\lambda_1(x-mt)} + \dots \quad (54)$$

$$\theta_E = c_1 + c_2 \left(1 - \frac{m}{\varepsilon} \lambda_1\right) e^{\lambda_1(x-mt)} + \dots \quad (55)$$

$$m = m_0 + \varepsilon \left(\frac{\alpha}{m_0} - \frac{2\alpha}{m_0 + \sqrt{m_0^2 + 4\alpha}} \right) + \dots \quad (56)$$

5. A boundary value problem

Assume a semi infinite substrate material heated with a time decaying source from the surface. The boundary conditions for the problem can be written as follows

$$\frac{\partial \theta_E}{\partial x}(0, t) = -I_0 e^{-k_1 t}, \quad \frac{\partial \theta_E}{\partial x}(\infty, t) = 0$$

$$\theta_E(x, \infty) = \theta_0, \quad \theta_L(x, \infty) = \theta_0 \quad (57)$$

The dimensionless source amplitude I_0 is related to the dimensional one \bar{I}_0 through the relation $I_0 = \bar{I}_0/(kdT_0)$. For the above boundary conditions, the approximate solutions are finally found to be

Table 1
Thermo-physical properties of gold at 300 K and other parameters used

Property	Numerical value
C_L	$2.5 \times 10^6 \text{ J m}^{-3} \text{ K}^{-1}$
C_E	$2.1 \times 10^4 \text{ J m}^{-3} \text{ K}^{-1}$
G	$2.6 \times 10^{16} \text{ W m}^{-3} \text{ K}^{-1}$
k	$315 \text{ W m}^{-1} \text{ K}^{-1}$
d	10^9 m^{-1}
I_0	31.75
k_1	0.2
T_0	300 K

$$\theta_E = \theta_0 - \frac{I_0}{\lambda_1} e^{\lambda_1 [x - (m_0 + \varepsilon m_1) t]} \quad (58)$$

$$\theta_L = \theta_0 - \frac{I_0}{\lambda_1 [1 - (m_1 + \frac{m_0}{\varepsilon}) \lambda_1]} e^{\lambda_1 [x - (m_0 + \varepsilon m_1) t]} \quad (59)$$

The dependence of the similarity parameter m on the decay rate is given by the relation

$$\lambda_1 m = k_1 \quad (60)$$

Gold is employed as substrate material and its thermo-physical properties as well as other parameters used in computations are given in Table 1. Fig. 1 shows electron and lattice

site temperatures obtained from the analytical solution and predicted from the numerical simulations as a function of time. Fig. 2 depicts the same comparisons as a function of distance. It can be observed that analytical solutions agree well with the numerical solutions. The small discrepancies may be due to the approximate nature of the analytical solutions. Nevertheless, they are negligibly small. Therefore, Figs. 1 and 2 indicate that the analytical solution has a sound base to predict the correct temperature rise in the electron and lattice sub-systems. It should be noted that a finite difference scheme is employed to discretize Eqs. (4) and (5). Grid independency and convergence are satisfied to secure the grid independent and converged results. The simulation conditions and parameters used are kept the same as those used in the analytical solutions. Further analytical solutions are plotted in Figs. 3–6. Fig. 3 shows the variation of electron temperature with time for three different locations. Since the heating is from the surface, the temperatures below the surface are lower. As time passes, the temperature tends to its constant value. Fig. 4 shows the variation of lattice site temperature with time for three different locations. As time passes, due to electron–phonon coupling, the lattice site temperature increases and tends to its constant value. Fig. 5

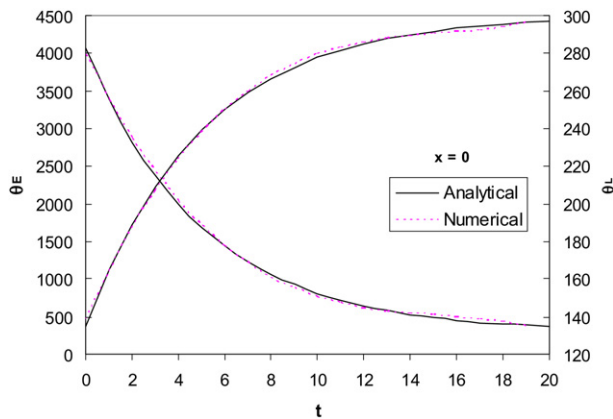


Fig. 1. Electron and lattice site temperatures versus time predicted numerically and obtained from the analytical solution ($x = 0$).

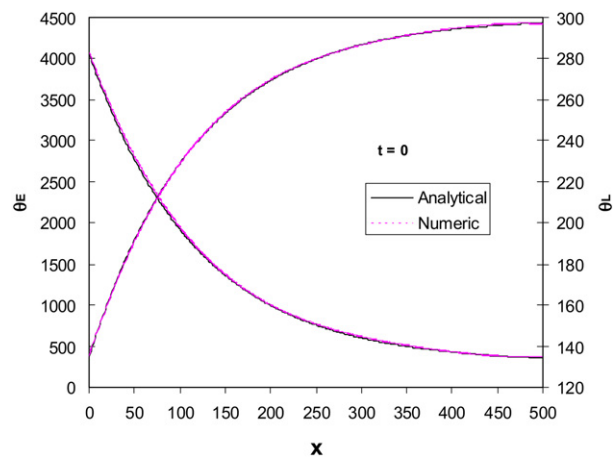


Fig. 2. Electron and lattice site temperatures versus distance predicted numerically and obtained from the analytical solution ($t = 0$).

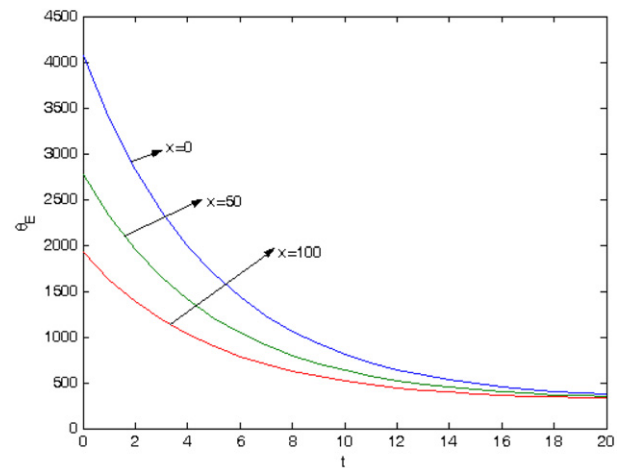


Fig. 3. Electron temperature versus time for different locations.

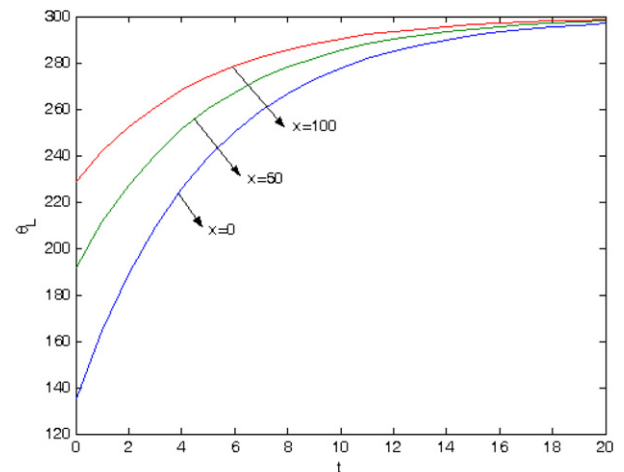


Fig. 4. Lattice site temperature versus time for different locations.

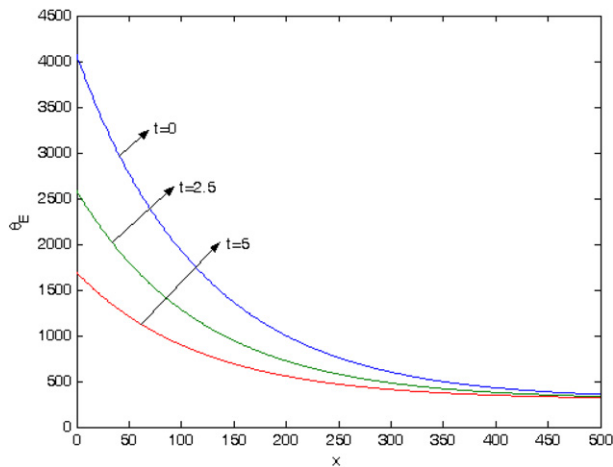


Fig. 5. Electron temperature versus distance for different time.

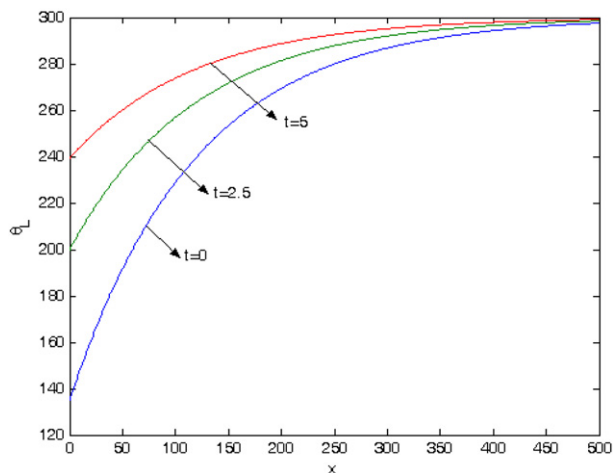


Fig. 6. Lattice site temperature versus distance for different time.

depicts electron temperature as a function of depth. Due to heating from the surface, electron temperatures are higher near to the surface. Heat is transferred to the lattice site from the electrons and as time passes the electron temperatures are lower. Finally Fig. 6 displays the lattice site temperature as a function of depth. Due to the heat transferred from the electrons, the lattice site temperatures increase in time.

6. Concluding remarks

Energy transfer equations in laser heating are considered. Equations are cast into a suitable dimensionless form. Symmetries of the equations are calculated using the Lie Group Theory. Using the symmetries, the partial differential system is transferred to an ordinary differential system. An approximate analytical solution is constructed using the strained parameters method, a perturbation technique. A boundary value problem with semi infinite substrate material and time decaying surface heating is considered. The electron and lattice site temperatures

and their behavior as time and depth varies are determined for the conditions considered. Approximate analytical solutions are verified by numerical solutions of the partial differential system.

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