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Bayesian estimation of thermophysical parameters of thin metal films heated by fast laser pulses ☆

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ABSTRACT

In this paper, we apply the Markov Chain Monte Carlo method, within the Bayesian framework, for the estimation of parameters appearing in the heat conduction model in metals under the condition of thermal non-equilibrium between electrons and lattice. Such non-equilibrium can be experimentally observed in a time scale of up to few picoseconds, during the heating of thin metal films with laser pulses of the order of femtoseconds. Simulated measurements containing random errors are used for the solution of the inverse problem. Results are presented for the simultaneous estimation of the electron–phonon coupling factor, the thermal conductivity and the heat capacity of the electron gas.

1. Introduction

The thermal nonequilibrium between electrons and lattice is an important phenomenon in the study of heat transfer in thin metal films subjected to fast laser pulses. The photon energy of the laser pulse absorbed by the electrons gives rise to a hot free-electron gas, which diffuses through the metal and heats up the lattice by electron–phonon collisions. For laser pulses of duration longer than the electron–phonon thermalization time, the electrons have enough time to establish equilibrium with the lattice, so that they have the same temperature. On the other hand, for laser pulses of the order of femtoseconds and in a time scale of up to few picoseconds, the variation of the lattice temperature is small compared to the electron temperature rise and thermal non-equilibrium can be experimentally observed [1–19].

For the current range of laser pulse durations used for the fast heating of thin metal films, the transient nonequilibrium temperatures of electrons, T_e, and lattice, T_l, can be described by the following parabolic model, which is written for a one dimensional problem [1–19]:

$$C_e(T_e)\frac{\partial T_e(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(K\frac{\partial T_e}{\partial x}\right) - G(T_e - T_l) + Q(x,t) \tag{1a}$$

$$C_l\frac{\partial T_l(x,t)}{\partial t} = G(T_e - T_l) \tag{1b}$$

In Eqs. (1a) and (1b), C_l and C_e are the lattice and the electron volumetric heat capacity, respectively, K is the thermal conductivity of the electron gas, $Q(x,t)$ is the source term resulting from the laser heating and G is the electron–phonon coupling factor, which controls heat transfer between electrons and lattice. Diffusion can be neglected in Eq. (1b), since heat is mainly carried by free electrons in metals during the nonequilibrium state duration. The electron–phonon coupling factor can be theoretically predicted, but inverse analysis techniques, such as the Levenberg–Marquardt method, can also be used for its estimation [8]. The thermal conductivity, the lattice volumetric heat capacity, and the electron–phonon coupling factor can be assumed as constant. For electron temperatures as those observed in experiments such as the one under analysis, the electron heat capacity is known to vary linearly with temperature in the form [8]:

$$C_e(T_e) = \gamma T_e. \tag{2}$$

In this communication we revisit the work presented in Ref. [8], which involved the estimation of the electron–phonon coupling factor, by extending the inverse analysis for the estimation of other parameters appearing in the two-temperature model given by Eqs. (1a), (1b), and (2). Another novelty of this communication is the estimation of these parameters within the Bayesian framework, by using the Markov Chain Monte Carlo (MCMC) method [20–24]. The solution of the inverse problem within the Bayesian framework is recast in the form of statistical inference from the posterior probability density, which is the conditional probability distribution of the unknown parameters given the measurements. The conditional probability of the measurements given the unknown parameters, which incorporates the related uncertainties, is called the likelihood. The information for the unknowns that reflects all the uncertainty of the parameters, without the information conveyed by the

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Nomenclature

C	volumetric heat capacity
G	electron phonon coupling factor
I	number of measurements
K	thermal conductivity of the electron gas
L	thickness of the medium
N	number of parameters
$\mathbf{P}$	vector of parameters
Q	heat source term resulting from the laser heating
R	reflectivity
T	temperature
Y	measurements, Eq. (7)
Greeks	
γ	coefficient for the linear variation of the electron heat capacity, Eq. (2)
σ	standard deviation
Subscripts	
e	electron gas
l	lattice
meas	measurements

measurements, is called the prior model. The formal mechanism to combine the new information (measurements) with the previously available information (prior) is Bayes' theorem [20–25].

2. Inverse problem

One dimensional geometry is considered for the inverse problem examined here. The metal film is assumed to be initially at uniform temperature and in thermal equilibrium, that is,

$$T_l(t_0) = T_e(t_0) = T_0, \tag{3}$$

where t_0 is the initial time. Heat losses at the film surfaces are neglected due to the short duration of the related experiment, that is,

$$\frac{\partial T_e}{\partial x} = 0 \quad \text{at } x = 0 \text{ and at } x = L = \text{thickness of the medium.} \tag{4a, b}$$

The source term $Q(x,t)$ resultant from the laser heating has the form [8]:

$$Q(x,t) = (1-R)I\alpha e^{-\alpha x} e^{-(t/t_p)^2} \tag{5}$$

where I is the maximum laser power flux, R is the surface reflectivity and t_p is the laser pulse duration. The absorption coefficient α is determined from the relation

$$\alpha = \frac{4\pi n'}{\lambda} \tag{6}$$

where λ is the wavelength of the heating laser and n' is the extinction coefficient, i.e., the coefficient of the imaginary part of the complex refractive index at the same wavelength.

For the *direct problem*, all the parameters appearing in the formulation of the physical problem under examination are considered known and the electron and lattice temperature fields can then be obtained. The solution of the direct problem in this work was obtained by finite differences. The calculations were started at time $t_0 = -3t_p$, when the heat source term is four orders of magnitude smaller than its maximum value, so that its effects can be neglected for previous times. For the calculation of the source term, the optical properties of the metal were assumed independent of light intensity, laser pulse duration and temperature.

The *inverse problem* considered here deals with the estimation of parameters appearing in the two-temperature model, given by Eqs. (1a)–(6), by using transient measurements of the temperature of the electron gas at the surface heated by the laser pulse. Such measurements can be obtained with a pump–probe setup. In such an arrangement, a laser beam (pump) is used to heat the sample, while another laser of much smaller intensity (probe) is used to measure changes in the metal's reflectivity [11–16]. The sample reflectivity changes with variations in the electron and lattice temperatures. However, in a time scale of up to few picoseconds the effects due to variations of the lattice temperature can be neglected, since the electron temperature rise is much larger than that of the lattice. Therefore, the measured data is taken in the form of the normalized temperature variation, which is given by:

$$Y_i = \frac{\Delta R(t_i)}{\Delta R_{max}} \tag{7}$$

where $\Delta R(t_i) = R(t_i) - R(t_0)$, for $i = 1,\ldots, I$, is the surface reflectivity variation at time t_i and $\Delta R_{\max}$ indicates the maximum reflectivity variation. We note that changes in the sample transmissivity can also be associated to changes in the electron temperature [11–16].

The solution of the inverse problem within the Bayesian framework is based on the following principles [20]: 1. All variables appearing in the mathematical formulation are modeled as random variables; 2. The randomness describes the degree of information concerning their realizations; 3. The degree of information concerning these values is coded in probability distributions; and 4. The solution of the inverse problem is the posterior probability distribution, from which distribution point estimates and other statistics are computed.

Bayes' theorem is stated as [20–25]:

$$\pi_{posterior}(\mathbf{P}) = \pi(\mathbf{P}|\mathbf{Y}) = \frac{\pi(\mathbf{P})\pi(\mathbf{Y}|\mathbf{P})}{\pi(\mathbf{Y})} \tag{8}$$

where $\mathbf{P}$ the vector of parameters in the two-temperature formulation, $Y^T = (Y_1, Y_2,\ldots, Y_I)$ is the vector containing the measured temperature variations, $\pi_{posterior}(\mathbf{P})$ is the posterior probability density, $\pi(\mathbf{P})$ is the prior density, $\pi(\mathbf{Y|P})$ is the likelihood function and $\pi(\mathbf{Y})$ is the marginal probability density of the measurements, which plays the role of a normalizing constant.

Point and confidence estimates from the posterior distribution typically require numerical integration. If the posterior probability distribution does not allow an analytical treatment, Markov Chain Monte Carlo (MCMC) methods are used to draw samples of all possible parameters, so that inference on the posterior probability is obtained through inference on the samples. A simple and robust implementation of the MCMC method is given by the Metropolis–Hastings algorithm [20–25]. The implementation of the Metropolis–Hastings algorithm starts with the selection of a proposal distribution $p(\mathbf{P}^*,\mathbf{P}^{t-1})$, which is used to draw a new candidate state $\mathbf{P}^*$, given the current state $\mathbf{P}^{t-1}$ of the Markov chain. Once the jumping distribution has been selected, the Metropolis–Hastings sampling algorithm can be implemented by repeating the following steps [20–25]:

1. Sample a *Candidate Point* $\mathbf{P}^*$ from a proposal distribution $p(\mathbf{P}^*,\mathbf{P}^{t-1})$.
2. Calculate the acceptance factor:

$$H = \min\left[1, \frac{\pi(\mathbf{P}^*|\mathbf{Y})p\left(\mathbf{P}^{t-1},\mathbf{P}^*\right)}{\pi\left(\mathbf{P}^{t-1}|\mathbf{Y}\right)p\left(\mathbf{P}^*,\mathbf{P}^{t-1}\right)}\right] \tag{9}$$