



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.

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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]:

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

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

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]:

$$C_e(T_e) = \gamma T_e. \quad (2)$$

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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