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Estimation of parameters of the dual-phase-lag model for heat conduction in metal-oxide-semiconductor field-effect transistors

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ABSTRACT

This communication deals with the solution of an inverse parameter estimation problem with the dual-phase-lag heat conduction model. The case considered involves the heating of a metal-oxide-semiconductor field-effect transistor, for time and spatial scales where the validity of the classical heat conduction model based on Fourier's Law, which considers an infinite speed of propagation of thermal waves, has been questioned. The Markov chain Monte Carlo method is applied for the estimation of the parameters within the Bayesian framework of statistics, by using simulated transient temperature measurements.

1. Introduction

Experimental evidences that Fourier's Law fails for small time and spatial scales, as well as for temperatures near the absolute zero (see, e.g. [1]), lead to the development of new constitutive equations that relate the heat conduction vector to the temperature gradient, in which the speed of propagation of thermal waves is finite [2–11]. The so-called dual-phase-lag model [7,8,10] considers the non-instantaneous effects between the heat conduction vector and the temperature gradient, in the form of relaxation times for these two quantities. Depending on the magnitudes of the relaxation times, the heat conduction vector and the temperature gradient can be synchronized, or either of one of these two vectors can be in advance with respect to the other. In general, when these newly developed constitutive equations are used, which consider the speed of propagation of thermal waves as finite, a hyperbolic equation results for modelling heat conduction, instead of the classical parabolic model obtained with Fourier's Law [2–11].

The technological advancement towards micro and nanoscales in electronic devices, often with large concentrated power, demands thermal design and analysis where heat conduction plays a major role. In particular, heat conduction in metal-oxide-semiconductor field-effect (MOSFET) transistors has been modelled using the dual-phase-lag constitutive equation [12–14], including boundary conditions that consider a temperature jump to simulate the phonon diffusion at the boundaries [15,16].

Inverse problems of heat transfer deal with the estimation of parameters or functions appearing in the mathematical models of thermal problems, by using measurements of dependent variables, like temperature, heat fluxes, radiation intensities, etc. [17–20]. Several works can be found in the literature regarding inverse analysis with mathematical models for heat conduction where the speed of propagation is considered as finite, including the dual-phase-lag model [21–26]. In this communication, we apply the Markov chain Monte Carlo method for the estimation of parameters appearing in the dual-phase-lag model for heat conduction in MOSFET transistors, by using simulated transient temperature measurements. The parameters are estimated within the Bayesian framework, where the information available before the measurements are taken is used in the inverse analysis in the form of prior statistical distribution functions [18–20,27,28]. The solution of the inverse problem within the Bayesian framework is obtained from the statistics of the posterior distribution function, which considers the prior distribution and the likelihood (statistical model for the measurement errors) through Bayes´ theorem. Samples of the posterior distribution were simulated in this communication with the Metropolis-Hastings algorithm [18–20,27–29]. Such algorithm is not presented here for the sake of brevity, but can be readily found in several references, including [18–20,27–29].

2. Physical problem and mathematical formulation

The physical problem considered here is based on that addressed in [13]. Fig. 1 illustrates the two-dimensional domain, which consists of a MOSFET transistor made of silicon ($\tau_q = 33.33$ ps, $\tau_T = 1.66$ ps, $k = 150$ $\text{Wm}^{-1}\text{K}^{-1}$, $C = 1.5 \times 10^6\ \text{Jm}^{-3}\text{K}^{-1}$, $\alpha = 10^{-4}\ \text{m}^2\text{s}^{-1}$, $\Lambda = 100$ nm [13,16]), with dimensions $L = 100$ nm and $l = 50$ nm. Heat is uniformly generated within the square region of side

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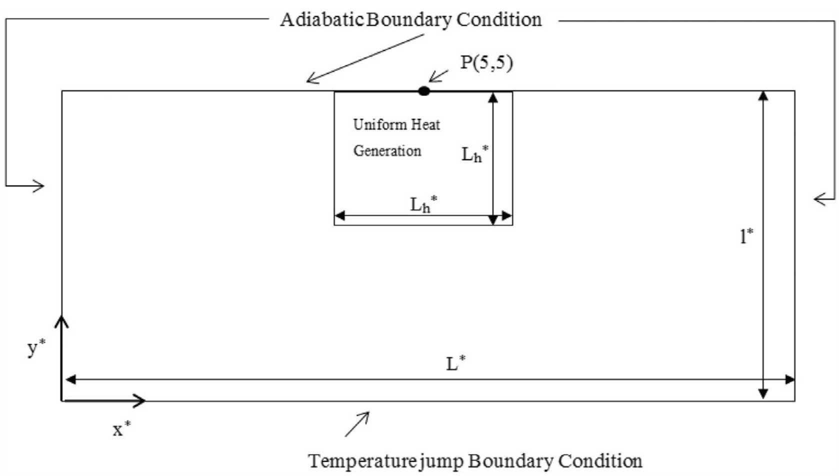

Fig. 1. Heat conduction in a MOSFET transistor.

$L_h = 10$ nm by Joule effect. The heat source is assumed to vary linearly from zero at time $t = 0$ to $Q_{max} = 10^{19}\,\mathrm{W/m^3}$ at $t = 10$ ps and kept constant afterwards. The top and lateral surfaces are thermally insulated, while the bottom surface is subjected to a temperature jump boundary condition to simulate the phonon diffusion at the boundary, where the surface is externally maintained at the temperature T_w. The initial temperature is uniform and taken as $T_0 = 300$ K.

The following dimensionless variables were utilized in this work:

$$T^* = \frac{T - T_0}{T_0}, \quad t^* = \frac{t\alpha_{ref}}{L_h{}^2}, \quad \tau_T{}^* = \frac{\tau_T}{\tau_{T_{ref}}}, \quad \tau_q{}^* = \frac{\tau_q}{\tau_{q_{ref}}}, \quad x^* = \frac{x}{L_h},$$
$$y^* = \frac{y}{L_h}$$
$$k^* = \frac{k}{k_{ref}}, \quad C^* = \frac{C}{C_{ref}}, \quad \alpha^* = \frac{\alpha}{\alpha_{ref}}, \quad Kn = \frac{\Lambda}{L_h}, \quad Q^* = \frac{L_h^2}{T_0 k_{ref}} Q \tag{1.a–k}$$

where the subscript *ref* denotes reference values, Kn is the Knudsen number, Λ is the mean free path of phonons, τ_q is the relaxation time for the heat flux vector and τ_T is the relaxation time for the temperature gradient. The reference values for the thermophysical properties were taken as those of silicon and $\tau_{T_{ref}} = \tau_{q_{ref}} = L_h{}^2/\alpha_{ref}$.

The mathematical formulation of the physical problem in dimensionless form is given by:

$$\frac{1}{\alpha^*}\frac{\partial T^*}{\partial t^*} + \frac{\tau_q^*}{\alpha^*}\frac{\partial^2 T^*}{\partial t^{*2}} = \left(\frac{\partial^2 T^*}{\partial x^{*2}} + \frac{\partial^2 T^*}{\partial y^{*2}}\right) + \tau_T^* \frac{\partial}{\partial t^*}\left(\frac{\partial^2 T^*}{\partial x^{*2}} + \frac{\partial^2 T^*}{\partial y^{*2}}\right) + \frac{Q^*}{k^*} + \frac{\tau_q^*}{k^*}\frac{\partial Q^*}{\partial t^*}$$
$$\text{in } 0 < x^* < L^*,\ 0 < y^* < l^*,\ \text{for } t^* > 0 \tag{2a}$$

$$\frac{\partial T^*}{\partial x^*} + \tau_T^* \frac{\partial}{\partial t^*}\left(\frac{\partial T^*}{\partial x^*}\right) = 0 \ \ at\ x^* = 0,\ 0 < y^* < l^*,\ \text{for } t^* > 0 \tag{2b}$$

$$\frac{\partial T^*}{\partial x^*} + \tau_T^* \frac{\partial}{\partial t^*}\left(\frac{\partial T^*}{\partial x^*}\right) = 0 \ \ at\ x^* = L^*,\ 0 < y^* < l^*,\ \text{for } t^* > 0 \tag{2c}$$

$$-\frac{k^*}{d_1 Kn}\frac{\partial T^*}{\partial y^*} - k^*\tau_T^* \frac{\partial}{\partial t^*}\left(\frac{\partial T^*}{\partial y^*}\right) + \tau_q^* \frac{1}{d_1 Kn}\frac{\partial T^*}{\partial t^*} + \frac{1}{d_1 Kn} T^* = \frac{1}{d_1 Kn} T_w^*$$
$$at\ \ y^* = 0,\ 0 < x^* < L^*, \quad \text{for } t^* > 0 \tag{2d}$$

$$\frac{\partial T^*}{\partial y^*} + \tau_T^* \frac{\partial}{\partial t^*}\left(\frac{\partial T^*}{\partial y^*}\right) = 0 \ \ at\ y^* = l^*,\ 0 < x^* < L^*,\ \text{for } t^* > 0 \tag{2e}$$

$$T^* = 0 \ \text{ in } 0 < x^* < L^*,\ 0 < y^* < l^*,\ \text{for } t^* = 0 \tag{2f}$$

$$\frac{\partial T^*}{\partial t^*} = 0 \ \ \text{in } 0 < x^* < L^*,\ 0 < y^* < l^*,\ \text{for } t^* = 0 \tag{2g}$$

where the properties were supposed constant, $d_1 = 0.061$ is the adjusting coefficient used in [13] and $T_w^* = \frac{T_w - T_0}{T_0}$.

3. Inverse problem

The inverse problem of interest deals with the simultaneous estimation of the vector of parameters

$$\mathbf{P} = [\alpha^*, \tau_q^*, \tau_T^*, Kn] \tag{3}$$

from the simulated temperature response at the point of maximum temperature in the substrate, located at $x^* = y^* = 5$ (P(5,5) in Fig. 1). The transient temperature readings contain errors, which are assumed to be additive, uncorrelated and normally distributed, with zero mean and known constant standard-deviation σ. The measurements were simulated by adding Gaussian errors to the solution of the direct problem at the point P(5,5) obtained with the reference values and with standard deviations of 5% and 10% relative to the maximum temperature at this point.

4. Results and discussions

Before estimating the parameters, the reduced sensitivity coefficients are examined. The reference values are used for such local analysis of the sensitivity coefficients, since the present estimation problem is nonlinear. The reduced sensitivity coefficients are obtained from the multiplication of the original sensitivity coefficients [17,19] by their corresponding parameter values. Hence, the reduced sensitivity coefficients for this problem can be compared to the temperature variation at the measurement position, in order to detect small magnitudes and linear dependence. For appropriate estimation of the parameters, the sensitivity coefficients should be linearly independent and with large magnitude [17,19]. The time variations of the sensitivity coefficients with respect to each parameter are presented by Fig. 2, together with the transient temperature at the measurement location. This figure shows that the sensitivity coefficients with respect to thermal diffusivity and to the relaxation times are of the same order of magnitude of the temperature variation. On the other hand, the magnitude of the sensitivity coefficient with respect to the Knudsen number is practically null. Such is the case because the Knudsen number appears in the temperature jump boundary condition at the bottom surface (eq. 2d), which does not significantly affect the temperatures at the measurement position during the time range analysed. The analysis of Fig. 2 also reveals that the sensitivity coefficients with respect to the thermal diffusivity and to the heat flux relaxation time tend towards linear dependence. On the other hand, the sensitivity coefficients with respect to the relaxation times are not linearly dependent and can be simultaneously estimated by using temperature measurements taken at the top surface of the transistor. In fact, the relaxation times are the quantities of most interest for this inverse analysis, because they cannot be measured by