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Comparison of Green's function solutions for different heat conduction models in electronic nanostructures

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ABSTRACT

This paper compares Green's function solutions obtained for different heat conduction models, such as the Fourier–Kirchhoff heat equation, the Cataneo–Vernotte wave equation and the Dual-Phase-Lag equation. The solutions are computed for a nanometer size one-dimensional benchmark structure with Neumann and Dirichlet conditions imposed at its boundaries. Particular attention was paid to the analysis of heat diffusion speed predicted by the considered heat conduction models and its dependence on the time lag values.

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1. Introduction

The continuous miniaturization of electronic devices and the increased speed of their operation rendered thermal simulation of electronic nanosystems an essential part of their analysis and design. For almost two centuries thermal processes were modeled employing the heat transfer theory proposed by Fourier in his famous work in 1822 [1]. The main shortcoming of this classic theory consists in the fact that it was derived based on the Fourier law stating that the heat flux is directly proportional to the temperature gradient, what leads to the parabolic Fourier–Kirchhoff (FK) equation and implies instantaneous propagation of temperature response throughout an entire analysis domain. For relatively large structures and long thermal analysis times this equation produces results consistent with measurements. However, during analyses of very rapid thermal processes or small structures, the temperature values predicted by this model do not agree any more with experimental data [2].

Consequently, alternative approaches were needed which would allow taking into account certain microscale effects in macroscale heat conduction models. The first effort to amend the classic Fourier theory was the modification proposed in 1958 independently by Cattaneo and Vernotte who postulated the existence of a heat flux delay with respect to temperature changes due to a relaxation time constant what lead to the Cattaneo–Vernotte (CV) hyperbolic wave equation [3,4]. This theory was further developed by Tzou [5], who introduced yet another time constant, which allowed temperature responses to be delayed with respect to heat flux changes, and formulated the Dual-Phase-Lag (DPL) equation. The applicability of these non-Fourier heat conduction models, summarized in [6], to the analysis of nanoscale electronic devices has been already demonstrated in [7,8].

Theoretically, more appropriate for analyses of thermal phenomena in nanostructures would be different microscopic models and approaches, such as the Boltzmann Transport Equation (BTE) or the Molecular Dynamics (MD) simulations reviewed in [9]. However, due to their high computational complexity and long simulation time, they can be employed only for analysis of individual devices and they do not seem appropriate for simulations at the system level. Fortunately, as demonstrated in [10], it is possible to derive the DPL equation from the BTE by relating microscopic model parameters to the heat flux and temperature relaxation time constants.

This paper, summarizing the authors' research on various heat conduction models, is organized as follows. The next section introduces briefly the considered heat conduction models. Then, for each model the construction of the Green's function (GF) for a one-dimensional benchmark structure is presented in detail. Next, the Green's function solution equations are formulated and the temperature distribution evolution in time is computed and compared for different models. In particular, the influence of the temperature and heat flux time delay values on the heat diffusion speed is investigated.

2. Comparison of heat conduction models

The original Fourier law of heat conduction assumes that the heat flux q is proportional to the negative gradient of temperature T. The introduction of the aforementioned heat flux and temperature relaxation time constants τ_q and τ_T leads to the modified

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Fourier law presented in Eq. 1. Compared to the Fourier law, this equation has two additional terms containing heat flux and temperature gradient time derivatives. The thermal conductivity k is the measure of heat conduction rate and the negative signs before terms involving the temperature gradient indicate that heat flows from regions of higher temperature towards cooler areas.

$$\tau_q \frac{\partial q}{\partial t} + q = -k\nabla T - k\tau_T \frac{\partial}{\partial t}(\nabla T) \tag{1}$$

Without internal heat generation and when model parameters do not depend on temperature, introducing the above relation into the energy balance performed for a unit volume the following DPL equation can be derived [11]

$$\alpha\, \tau_T \frac{\partial}{\partial t}(\nabla^2 T) + \alpha \nabla^2 T = \frac{\partial T}{\partial t} + \tau_q \frac{\partial^2 T}{\partial t^2} \tag{2}$$

The parameter α is called thermal diffusivity. Compared to the FK heat equation, in the DPL equation two new terms proportional to the relaxation time constants appear. They contain the second time derivative and the mixed third order derivative of temperature. The latter term, in turn, distinguishes the DPL equation from the CV one. For the convenience of mathematical analyses, the DPL equation is considered sometimes in its dimensionless form where the temperature rise Θ over the ambient temperature fulfills the following relation [11]:

$$B \frac{\partial}{\partial \eta}(\nabla^2 \Theta) + \nabla^2 \Theta = 2\frac{\partial \Theta}{\partial \eta} + \frac{\partial^2 \Theta}{\partial \eta^2} \tag{3}$$

with the dimensionless time η and the constant B defined as

$$\eta = \frac{t}{2\tau_q}; \quad B = \frac{\tau_T}{2\tau_q} \tag{4}$$

The CV wave equation is obtained from Eq. 3 when B equals to 0 whereas the FK relation is obtained when parameter B equals to 0.5. It is worth mentioning that the latter condition implies that the FK equation can be obtained for any value of the relaxation time constant greater than zero as long as τ_q and τ_T are equal each other.

3. Construction of Green's functions

This section will provide a brief theoretical introduction to Green's functions. This will be followed by the description of the benchmark structure and the presentation of the appropriate GFs for each of the heat conduction models considered in this paper.

3.1. Theoretical introduction to Green's functions

Green's functions are versatile mathematical tools suitable for obtaining solutions of linear partial differential equations [12,13]. A Green's function for the heat equation can be regarded as a temperature response in a point x at time t caused by instantaneous heat generation in a point x' at time τ. Thus, in order to compute the temperature response in time, it is enough to integrate a GF over the entire volume and time where heat is generated. Alternatively, a GF describes the temperature distribution at a point x in time t due to an initial temperature rise at a point x'. Then, the entire temperature field can be computed by integrating over the entire domain a GF evaluated at the starting time of the analysis [14].

Particular GFs depend only on problem geometry and applied boundary conditions. Thus, using the same GF the total temperature rise can be computed as the superposition of individual temperature rises caused by different factors, such as the initial temperature distribution, the internal heat generation and the non-homogeneous boundary conditions.

Green's functions can be derived using different methods, e.g., the method of images, the Laplace transform method or the Fourier separation of variables method yielding solutions in different, but mathematically equivalent, forms. Generally, the first two methods produce series solutions which are rapidly convergent for short times whereas the Fourier method solutions are better convergent for large times.

3.2. Benchmark structure

The one-dimensional benchmark structure analyzed in this paper, shown in Fig. 1, is a thin slab of a thickness d equals to 10 nm. This structure is heated from the left side by the heat flux q and ideally cooled at the right one where the isothermal boundary condition is imposed. This structure could resemble a real electronic nanostructure, whose lateral dimensions are typically much larger than its thickness. The choice of this test structure was made expressly to render possible the comparison of obtained results with the previous simulations carried out by the authors employing the FK heat equation and CV wave equation in [15,16] respectively.

3.3. Green's functions for the benchmark structure

Green's functions are obtained as solutions of an auxiliary equation which is exactly the same as the original one; with the only exception that its boundary conditions are of the same type but homogenous ones. Thus, the GFs for the three heat conduction models considered here can be found applying to the benchmark structure the adiabatic condition on the left boundary and assuming that the temperature at the right boundary equals to 0, i.e. the same as the original boundary condition [14].

Then, since the analyses published in [15] showed that even for times of the order of picoseconds and nanometer dimension the Fourier separation of variables solution method is still computationally efficient, the GF obtained using this method can be used for the FK equation. This function, evaluated at the nonhomogeneous boundary at $r' = 0$, has the form of the following infinite series:

$$G(x, t \mid 0, \tau) = \frac{2}{d} \sum_{n=1}^{\infty} \exp\left(-\beta_n^2 \alpha (t-\tau)\right) \cos\left(\beta_n x\right) \tag{5}$$

Although theoretically the number of series components is infinite, in practice it is enough to compute only several tens of components to attain the four digit accuracy. The eigenvalues β_n appearing in the formula can be found applying the specific boundary conditions and they are equal to $\pi\,(n - 1/2)$. For different time instants this function will be plotted and analyzed later on together with the discussion concerning the DPL equation.

On the other hand for the CV wave equation the GF obtained with the Fourier solution method is slowly convergent and it requires taking into account thousands of series terms, hence it is more convenient to use the GF obtained using the method of images. This function, shown in Eq. 6, can be expressed as the product of an exponential function and the zeroth order modified

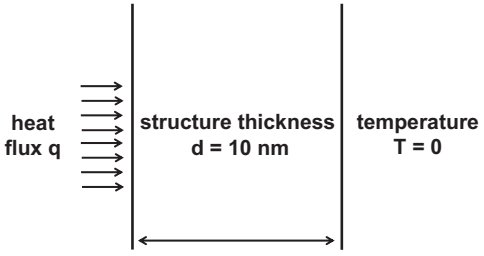

Fig. 1. One-dimensional benchmark structure with imposed boundary conditions.

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