Application of Dual-Phase-Lag Model for Thermal Analyses of Electronic Nanostructures

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ABSTRACT

This paper introduces the dual-phase-lag differential equation as a possible new candidate to model heat transfer processes in nanostructures. The main advantage of this equation is that, depending on the particular choice of the equation parameters, it encompasses all the widely applied models, i.e. the standard Fourier-Kirchhoff heat equation or the Cattaneo-Vernotte hyperbolic equation. The analyses presented here are based on the solutions of the dual-phase-lag equation obtained with the Green's function method for a one-dimensional benchmark structure.

Keywords: nanoscale heat transfer, dual-phase-lag equation, Green's functions

1 INTRODUCTION

The continuous miniaturization of electronic devices and the increase of their operating speed has brought the classic, almost two-century old [1], Fourier theory of heat conduction to the limits of its applicability. The main fault of the Fourier heat transfer theory results from the fact that it assumes that the heat flux is directly proportional to the temperature gradient implying instantaneous propagation of temperature response throughout an entire structure.

Consequently, the first amendment made to the Fourier heat conduction law by Cattaneo and Vernotte postulated the existence of heat flux delay with respect to temperature changes due to some time relaxation constant [2]-[3]. This theory was further developed by Tzou [4], who introduced yet another time constant allowing temperature responses to be delayed with respect to heat flux changes. All these modifications led to the Dual-Phase-Lag (DPL) differential equation describing thermal processes occurring in solids. More information on these macroscopic heat conduction models can be found in [5].

Theoretically, more appropriate for analyses of thermal phenomena in nanostructures are different microscopic models and approaches, such as the Boltzmann transport equation or the molecular dynamics simulations, reviewed in [6]. However, they can be employed only for analysis of individual devices but they are not suitable for analysis of larger nanosystems. Fortunately, as demonstrated in [7], it is possible to relate the microscopic models to the DPL equation, which will be analyzed in detail throughout the remainder of this paper.

The following section of this paper describes the DPL equation. Then, its Green's function solution for a one-dimensional benchmark structure is discussed. In particular, the influence of the temperature and heat flux time delay values on the heat diffusion speed is investigated. Finally, the temperature solutions obtained for various equation parameter values are compared.

2 DUAL-PHASE-LAG EQUATION

The dual-phase-lag equation is based on the modified heat conduction law, according to which the temperature T in a material of thermal conductivity k is related to the heat flux q by the following equation [4]:

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

Compared to the standard Fourier law, this equation has two additional terms including the relaxation time constants τ_q and τ_T, which are to model the respective heat flux and temperature delays. Thus, the modified heat conduction law contains terms depending on the heat flux time derivative and the mixed space and time derivative of temperature.

Without any internal heat generation and when model parameters do not depend on temperature, performing the energy balance for a unit volume the dimensionless DPL partial differential equation can be derived [8]:

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

This time again, compared to the classic heat equation two new terms proportional to the relaxation time constants appear. They contain the second time derivative and the mixed third order derivative of dimensionless temperature Θ. The constant B equals $\tau_T / (2\tau_q)$ and the dimensionless time η is $t / (2\tau_q)$.

The hyperbolic Cattaneo-Vernotte (CV) heat conduction equation is obtained when B equals 0 whereas the standard Fourier-Kirchhoff (FK) model is obtained when parameter B equals 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.
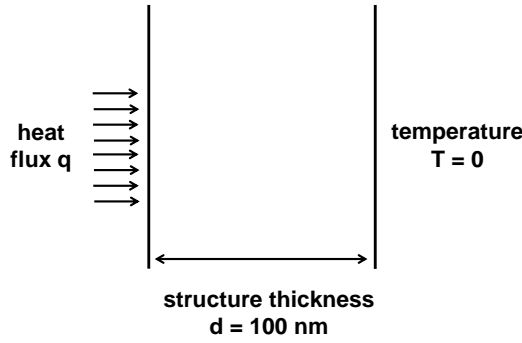
Figure 1: Benchmark structure.

Figure 2: Time evolution of Green's functions.

3 DPL EQUATION GREEN'S FUNCTIONS FOR THE BENCHMARK STRUCTURE

For simple geometries, the DPL equation can be solved employing the analytical Green's function (GF) method. These functions can be regarded as temperature responses at a coordinate x at time t due to the instantaneous heat generation at the location x' at time t'. The GF method renders possible the computation of temperature solutions for different boundary conditions performing adequate integration but still using the same GF, which depends only on the geometry of a particular structure.

The analyses presented in this paper are carried out for a thin one-dimensional slab of thickness d equal to 100 nm heated on one side by a heat flux q and cooled on the other side by the imposed isothermal boundary condition. This structure, shown in Fig. 1, might resemble a real electronic nanostructure, whose lateral dimensions are typically much larger than its thickness.

Generally, as shown in Eq. 3, a Green's function G for the DPL equation could be split into two parts, where the second component is proportional to the dimensionless time derivative of the first one. The dimensionless coordinates r and r' are obtained from their dimensional counterparts x and x' dividing them by $2\,(\alpha\,\tau_q)^{0.5}$, where α is material thermal diffusivity, and the dimensionless time τ is equal to $t'/(2\,\tau_q)$. Due to the limited space of this publication, the exact construction of the GFs will not be described here but the derivation of the formulas can be found for a general case in [8] and for the particular benchmark structure in [9].

$$G\left(r,\eta/r',\tau\right) = G_x\left(r,\eta/r',\tau\right) + \frac{1}{2}\frac{\partial G_x\left(r,\eta/r',\tau\right)}{\partial \eta} \qquad (3)$$

The main goal of the present research was to investigate how the heat diffusion speed depends on the value of the parameter B, i.e. the ratio of the relaxation time constants τ_q and τ_T. For the computations, three different values of the parameter B were assumed: 0.1, 0.5 and 2.0. The GF values computed for time instants of 500 fs, 2 ps and 100 ps are represented in Fig. 2 with dotted, dashed and solid lines respectively. The colors denote a particular value of B.
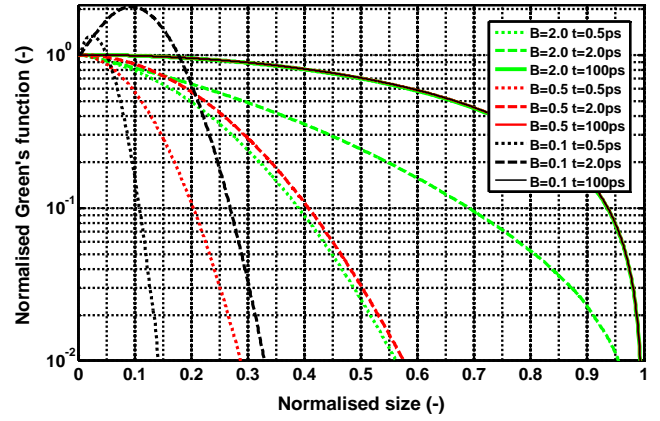
Since for different time instants and parameter B values the GFs have different magnitudes, in order to make the comparison between the curves possible each curve was normalized with respect to its value at the left boundary and plotted on the logarithmic scale. Additionally, the values on the horizontal axis were normalized with respect to the structure thickness.

Analyzing the curves in the figure, one can notice that the heat diffusion speed significantly depends on the value of the parameter B and the increase of the relaxation time constant τ_T reduces the diffusion time. When τ_T is smaller than τ_q ($B < 0.5$), i.e. if heat diffuses slower than for the classic FK equation, at short diffusion times the maximum of the GF occurs inside the structure, what might produce instantaneous transient temperature rise values higher than in the steady state (for details refer to [10]). Although the transient temperature values might visibly differ for various values of B, all the curves eventually converge to the same steady state limits.

The dependence of heat diffusion time on the parameter B value was investigated in more detail. The results of these analyses are presented in Fig. 3. The diffusion time was defined here as the time required to noticeably increase, i.e. by 1% of temperature rise value at structure surface, the temperature in the middle of the structure.
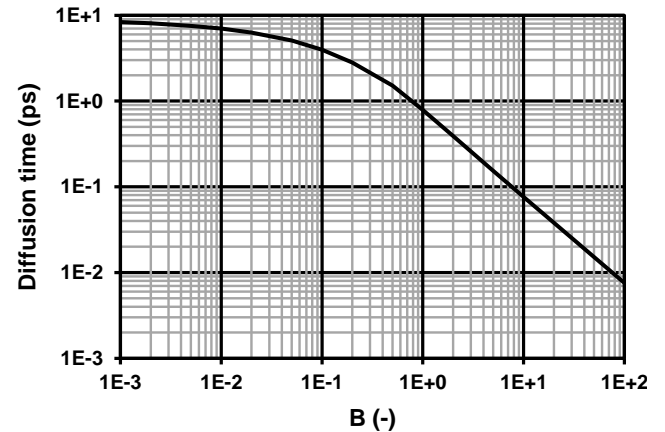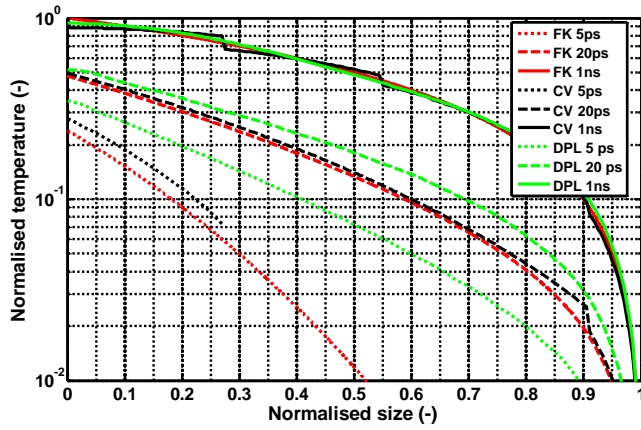

Figure 3: Dependence of diffusion time on parameter B.

Figure 4: Temperature time evolution.

When B equals 0, the diffusion speed corresponds to the one predicted by the classic hyperbolic CV equation, i.e. $(\alpha / \tau_q)^{0.5}$ (for most solids this value is of the order of a few thousands of meters per second) and the heat diffusion time slightly exceeds 9 ps. Then, the heat diffusion time visibly decreases and for the FK equation ($B = 0.5$) it amounts to around 1.5 ps to reach just 7.6 fs for $B = 100$.

4 TEMPERATURE SOLUTION

Given the GF for the analyzed structure, it is possible to compute the temperature distribution at any time instant by performing time integration of the GF as shown in Eq. 4. Taking into account that the only factor contributing to the overall temperature rise is the nonhomogeneous boundary condition of the second kind at the left side, the GF needs to be evaluated only at r' equal to 0 [8].

$$
\Theta(r,\eta) = \frac{1}{4d} \int_{\tau=0}^{\eta} [G_x(r,\eta/0,\tau) + \\
+ 2B \frac{1}{2} \frac{\partial G_x(r,\eta/0,\tau)}{\partial \eta}] \, d\tau
$$

(3)

The temperature distribution in the structure computed according to the above formula for the FK model ($B = 0.5$), the CV model ($B = 0$) and the DPL model (for $B = 2$) are compared in Fig. 4. This time the values on the vertical axis were normalized with respect to the maximal steady state temperature rise, i.e. $(q\, d) / k$.

For the classic FK heat equation after 5 ps the surface temperature reaches one-fourth of the steady state value and the temperature response develops already in a half of the structure. After 20 ps the temperature response is already fully developed and the surface temperature reaches the half of its steady state value. All the computed curves match exactly those given in [11], where the convergence of GFs for the FK equation was investigated.

On the other hand, for the CV hyperbolic heat equation the heat diffuses much slower and after 5 ps the wave front reaches only one-fourth of the structure. After 20 ps, i.e. just after the first reflection of the heat wave from the right boundary, the temperature distribution profile is close to the FK solution only with a slight temperature 'jump' resulting from the heat wave reflection. Unlike in the case of thinner structures [12], neither instantaneous negative temperature rise values are observed nor do temperature transient values exceed significantly the steady state ones.

For the DPL model with $B = 2$ the temperature response develops much faster and the surface temperature reaches one-third of the steady state value after 5 ps. Nevertheless, in spite of the fact that the speed of the transient thermal processes strongly depends on the value of parameter B, all curves eventually converge in less than 100 ps to the same steady state curve which is a straight line when applying linear scale to both axes.

5 CONCLUSIONS

This paper presented the DPL equation and discussed the possibility of applying this equation to modeling of heat transfer processes at nanoscale. In particular, the usefulness of the Green's function method for the solution of the DPL equation was demonstrated. Obviously, for more complex problem geometries some numerical solution method could be used.

The potential attractiveness of the DPL model originates from the fact that this equation not only includes as its particular cases other equations widely used for modeling of thermal processes, such as the FK heat equation or the CV wave equation, but it could be also fitted to existing experimental data or some microscopic models such as the Boltzmann transport equation. Although dynamic thermal responses differ significantly for all the considered models, finally they converge to the same steady state temperature distribution.

The simulations presented in this paper demonstrated that in the DPL equation the speed of heat diffusion could be efficiently controlled by adjusting the ratio of relaxation time constants, i.e. the value of parameter B. In particular, the simulations showed that the lowest speed is obtained for the CV wave equation model ($B = 0$) and it increases with the value of this parameter.

From the practical applicability point of view, when modeling electronic nanosystems it should be expected that the range of useful values of parameter B is well over the one for the FK model, i.e. 0.5. Although the hyperbolic wave equation might be appropriate for modelling of short laser pulse heating [13] or similar thermal processes but the experimental data published in [4] and [14] suggest rather that in semiconductors and metals the values of parameter B for nanoscale devices even exceed 100 what leads to the phenomenon called by certain authors the 'superdiffusion' of heat.

REFERENCES

[1] J. B. J. Fourier, "Théorie analytique de la chaleur," Firmin Didot, 1822.

[2] C. Cattaneo, "Sur une forme de l'équation de la chaleur éliminant le paradoxe d'une propagation instantanée," Comptes Rendus Académie Scientifique, 247, pp. 431-433, 1958.

[3] P. Vernotte, "Les paradoxes de la théorie continue de l'équation de la chaleur," Comptes Rendus Académie Scientifique, 246, pp. 3154-3155, 1958.

[4] D. Y. Tzou, "Macro- to Microscale Heat Transfer: The Lagging Behavior," Taylor & Francis, 1997.

[5] L. Wang, X., Zhou, X. Wei, "Heat Conduction: Mathematical Models and Analytical Solutions, Springer, 2008.

[6] D. Cahill, W. K. Ford, K. E. Goodson, G. Mahan, A. Majumdar, H. J. Maris, R. Merlin, S. Phillpot, "Nanoscale thermal transport," Journal of Applied Physics, 93, pp. 793-818, 2003.

[7] M. Xu, and L. Wang, "Dual-phase-lagging heat conduction based on the Boltzmann transport equation," International Journal of Heat and Mass Transfer, 48, pp. 5616-5624, 2005.

[8] R. Al-Khairy, "Green's function solution for dual-phase-lag heat equation," Applied Mathematics, 3, pp. 1170-1178, 2012.

[9] M. Janicki, M. Zubert, A. Samson, T. Raszkowski, A. Napieralski, "Green's function solution for dual-phase-lag heat conduction model in electronic nano-structures," Proc. of 31st SEMI-THERM, pp. 95-98, 2015.

[10] B. Vermeersch, G. De Mey, "Non-Fourier thermal conduction in nanoscaled electronic structures," Analog Integrated Circuits & Signal Processing, 55, pp. 197-204, 2008.

[11] M. Janicki, M. Zubert, and Andrzej Napieralski, "Convergence of Green's function heat equation solutions in electronic nanostructures," Proc. 21st MIXDES, pp. 285-288, 2014.

[12] M. Janicki, M. Zubert, A. Napieralski, "Green's function solution of hyperbolic heat equation suitable for thermal analysis of electronic nanostructures," Proc. 20th THERMINIC, p. 5-06, 2014.

[13] D. W. Tang, N. Araki, "Analytical solution of non-Fourier temperature response in a finite medium under laser-pulse heating," Heat and Mass Transfer, 31, pp. 359-363, 1996.

[14] B. Vermeersch, J. Carrete, N. Mingo, A. Shakouri, "Superdiffusive heat conduction in semiconductor alloys: Theoretical foundations," Physical Review B, 91, 085202, 2015.