Lodz University of Technology

Faculty of Electrical, Electronic, Computer and Control Engineering

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Abstract of Doctoral Dissertation

Numerical modelling of thermal phenomena in nanometric semiconductor structures

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Nowadays, heat distribution modeling is one of the most importants stages in the design process of integrated circuits and systems. Properly conducted thermal analysis is extremely important in the context of the correct design of the integrated circuit, it allows the analysis of critical places of the integrated circuit that have an impact on possible electro-thermal couplings, stability of operation and their life time. This analysis has a utilitarian character and becomes necessary in the case of structures dedicated to special applications in industry, medicine and military applications. The degree of complexity of thermal analyses depends on many factors, among which the type of the analyzed electronic structure (e.g. analogue and digital systems) can be mentioned, the technological process in which the structure has been designed (e.g. classical CMOS, MEMS, nanotubes, etc.), and a model that is used to determine the temperature distribution on the surface or inside the considered system.

The most commonly used model describing the heat flow is the Fourier-Kirchhoff (FK) model. However, as the results of the research show, in the case of nanometric electronic structures the more appropriate choice is the Dual-Phase-Lag thermal model (DPL), which is the subject of this thesis. Research on properties and various aspects of the use of this model were carried out, among others, as part of some research projects, in which the author has participated in as a contractor or a manager.

The purpose of the research conducted in relation to mentioned projects and the aim of this thesis was to develop algorithms aimed at simplifying the use of the Dual-Phase-Lag model and to reduce the time needed to obtain the results of the temperature distribution simulations based on the analyzed nanometer electronic structures.

The following theses have been formulated in this dissertation:

Thesis 1. It is possible to develop a one-dimensional differential scheme of the Dual-Phase-Lag model that allows for effective numerical approximation of heat flow in the considered electronic structures.

Thesis 2. It is possible to use the Grünwald-Letnikov derivative of fractional order for approximation and numerical simulation of the Dual-Phase-Lag equation in problems related to modeling of thermal phenomena in the heat generation sources for nanometric electronic structures.

Thesis 3. It is possible to develop a differential scheme for the Dual-Phase-Lag model and to develop a model order reduction algorithm using the proposed differential scheme, which allows for a significant acceleration of the numerical temperature simulations in analyzed semiconductor nanometric structures.

Thesis 4. The change of the temperature time lag τ_T constant in the Dual-Phase-Lag thermal model generates greater differences in the dynamics of the temperature rise in the nanometric electronic structures analyzed in the work than the analogue change of the heat flux time lag τ_q constant.

To prove the truth of the above theses was connected with the implementation of the following **interdisciplinary tasks**:

1. analysis of theoretical mathematical models describing the heat flow in electronic structures,
2. analysis of the numerical methods for solving partial and ordinary differential equations of different orders,
3. development of the original approximation scheme for the Dual-Phase-Lag model in one-dimensional Euclidean space,
4. development of the original algorithm for determining the temperature distribution and heat flux density based on the application of the Dual-Phase-Lag heat conduction model in nanometric electronic structures considered in one-dimensional Euclidean space,
5. analysis of theoretical mathematical models enabling the obtainment of the fractional order derivatives,
6. development of the original approximation scheme for the Dual-Phase-Lag model in two-dimensional Euclidean space,
7. development of original algorithms for determining the temperature distribution in nanometric electronic structures using the mathematical models newly developed by the author of the dissertation, thanks to which it is possible to approximate the Dual-Phase-Lag thermal model based on the use of a modified Fourier-Kirchhoff model, in which instead of a time, space or both time and space derivatives of the temperature function, the definition of fractional Grünwald-Letnikov derivative is used in the case of two-dimensional Euclidean space,
8. analysis of possibilities of reduction of the differential equations system describing the Dual-Phase-Lag model,

9. development of the original approximation scheme for the Dual-Phase-Lag model in three-dimensional Euclidean space,
10. development of original algorithms enabling the Dual-Phase-Lag model order reduction, based on the Krylov's subspace method, to approximate the temperature distribution in the case of one-, two- or three-dimensional Euclidean space,
11. development of an algorithm enabling the analysis of the influence of Dual-Phase-Lag thermal model parameters on the temperature distribution in selected prototyped nanometric electronic structures,
12. analysis of simulation results, computational complexity and convergence of developed algorithms.

The way of achieving above objectives as well as results related to them, are discussed in detail in chapters 2-7 of this dissertation.

In chapter 2, which is the first of two theoretical chapters, task 1 from the list above was implemented. This chapter contains an introduction to the issue of the heat exchange in electronic structures. It contains descriptions of several selected mathematical models that enable description of the heat distribution, with particular emphasis on the Dual-Phase-Lag model and the Fourier-Kirchhoff model.

In chapter 3, stating the second theoretical chapter, task 2 was carried out. This section contains several selected methods for solving partial and ordinary differential equations and selected methods for transforming partial differential equations into ordinary ones. In addition, selected basic types of boundary conditions were described and a brief characterization of initial conditions also was made.

Chapters 4-6 consist of both theoretical considerations and the practical parts. Chapter 4 contains detailed descriptions of the implementation of tasks 3, 4 and 12. It contains the considerations regarding the preparation of the approximation scheme for the Dual-Phase-Lag problem in one-dimensional Euclidean space and describes the algorithm by which it is possible to determine the temperature distribution and heat flux density in selected structures based on prepared approximation scheme. The presented considerations were supplemented with an analysis of the convergence of the proposed approach and the estimation of its computational complexity. In addition, in this chapter **Thesis 1** has been proved.

Chapter 5 presents the characteristics and results obtained during implementation of tasks 5, 6, 7 and 12. The discussed chapter presents theoretical considerations concerning mathematical models describing selected types of fractional derivatives. In addition, approximation schemes were prepared for Fourier-Kirchhoff and Dual-Phase-Lag models in two-dimensional Euclidean space. In addition, three new mathematical models based on the Fourier-Kirchhoff model were developed, in which instead of using the classical definition of the time, space or both time and space derivatives of the temperature function, the fractional Grünwald-Letnikov derivatives have been used. This chapter also specifies the formulas approximating the value of the analyzed fractional order derivatives depending on the corresponding parameters of the Dual-Phase-Lag model. In relation to all developed models, the accuracy of their adjustment to the data obtained from the simulation was analyzed and their applicability ranges as well as the generated error levels were determined. Based on the presented analyzes, **Thesis 2** has also been proven in section 5.

Section 6 includes descriptions and results obtained in relation to implementation of tasks 8, 9, 10 and 12. This chapter analyzes the Krylov's subspace method and its numerical implementation, thanks to which it is possible to reduce the order of the Dual-Phase-Lag differential equations, and thus to shorten the time needed to obtain the results of the simulation of the temperature distribution in the analyzed electronic structures. Chapter 6 also contains a description of the approximation scheme prepared for Fourier-Kirchhoff and Dual-Phase-Lag models in three-dimensional Euclidean space. This section analyzes the compatibility of the simulation results using non-reduced and reduced thermal models. In addition, the time complexity of algorithms using both mentioned types of thermal models was estimated and the error of approximation of the non-reduced Dual-Phase-Lag model by its reduced version was analyzed in one-, two- and three-dimensional Euclidean space. The results described in chapter 6 prove the **Thesis 3** of this dissertation.

It is worth highlighting that task 12 was carried out in the case of each developed algorithm presented in chapters 4-6.

The last chapter, containing practical results from conducted research, is chapter 7, in which the task 11 was carried out. The first part of this chapter presents examples of numerical modeling of the heat distribution in selected, existing or prototyped, nanometric electronic structures. In the second part of section 7, the analysis of the influence of changes of the Dual-Phase-Lag model parameters on the change of the temperature distribution in selected semiconductor structures was made. The results research described in this section prove the **Thesis 4** of this dissertation.

The last chapter of the thesis is section 8, in which a short summary of the research described in this dissertation was made.

This dissertation has an interdisciplinary character due to included considerations on IT, electronic, mathematical and physical issues.