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DUAL-PHASE-LAG HEAT EQUATION MODELLING OF THE NANOELECTRONIC STRUCTURES TEMPERATURES

Summary

This paper presents the comparison of temperature distributions in nanometric multilayer electronic structure obtained using Fourier-Kirchhoff and Dual-Phase-Lag models. The numerical solution has been obtained using FEM method. Simulation results are precisely described and discussed. Thermal model, which is more relevant for nanometric electronic structures, is indicated.

Keywords and phrases: Dual-Phase-Lag, heat transfer, Fourier-Kirchhoff solution, heat equation, nanoelectronics, temperature distribution

1. Introduction

The newest trends in designing of the modern electronic appliances indicate that the dimensions of such devices should be as small as possible. These trends are the result of the customers expectations connected to the convenience and ease of use. These elements, in turn, are related to the light weight of the mentioned devices, their small size, intuitiveness of use and the reliability of their operation. All of the mentioned factors have the big influence on the utility of the appliances and they often decide about their commercial success which leads to financial benefits for the manufacturers and to customers satisfaction.

However, there is not possible to achieve the high level of the reliability of electronic devices without the proper estimation of the temperature distribution inside the analyzed appliances. As it turns, the temperature has the most meaningful influence on the appropriate operation of the electronic device. Moreover, the temperature is the factor which causes the biggest number of malfunctions of electronic devices [1]. There are some important reasons which have the significant influence on the thermal damages of the electronic devices:

- miniaturization of electronic appliances,
- improper cooling conditions,
- high operating frequencies,
- defective construction of the device escalating accumulation of the heat inside the device,
- inappropriate approach to modelling the temperature distribution in investigated appliance,
- erroneous estimation of the temperature rises during the operation of the device.

The first of the reasons listed above is connected with the difficulties in heat dissipation. Small volumes of the modern appliance cause that the particular elements of the integrated circuits are implemented closer to each other. Thus, the free airflow is straitened. Therefore, the more intensive temperature rises are observed.

The second reason of the malfunctions caused by the listed thermal problems is related to the impossibility of implementation of efficient cooling in tiny structures. Their dimensions preclude the installation of the big heat sinks or other structures which provide the air cooling. Due to this fact, the heat generated during the device operation can be dissipated in insufficient way.

The next reason from the list above is a result of the need for the structures which are modern, fast and highly productive. This fact causes increase of the operating frequency of newly designed electronics. However, it also means that the temperature which is generated is higher than in the case in the older structures. One of the solutions of this problem is the reduction of the operating frequency but the efficiency of analyzed structure will be also reduced.

Another reason mentioned in the list presented previously is a result of errors made during the designing process. The most important of them is failure to take account the fact that in some parts of the structure more heat is generated. Apart from that, it is also very important to identify all paths of the heat dissipation in order to manage the temperature distribution in the proper way.

On the other hand, most of the problems mentioned previously can be solved by the correct modelling of the temperature distribution in analyzed structure. The thermal model should taking into consideration all factors which have the big influence on the temperature rise. In the case when some significant factors are neglected, the thermal simulations usually bring the meaningful errors of the estimation of the device temperature during its operation. Thus, this part of the research seems to be one of the most important development step in modern electronics designing process. The analysis of the simulation results allows taking into consideration the physical phenomena influencing on the temperature rises, avoiding designing errors and improving the reliability of the designed devices.

Thus, the choice of the appropriate thermal model is needed. One of the commonly used thermal models in current thermal simulators is Fouriers approach. It is based on the law which has been established in the first half of the nineteenth century by J. B. J. Fourier. This law, also known as the Fourier law, informs that the value of the heat flux is equal to negative temperature gradient multiplied by the thermal conductivity of the analyzed material [2]. The further development of the heat conductions problems allows establishing the Fourier-Kirchhoff equation based on the previously mentioned Fouriers law. Both the Fouriers law and the Fourier-Kirchhoff equations can be described in the form of the equations 1 and 2:

$$q(x,t) = -k \cdot \nabla T(x,t) \tag{1}$$

$$c_{vs}\frac{\partial T\left(x,t\right)}{\partial t} = -\nabla q\left(x,t\right) \tag{2}$$

The first equation represents the mathematical description of the Fouriers law while the second one reflects the Fourier-Kirchhoff heat equation. Moreover, the symbols used in described systems of equations have the meanings presented in the Table 1.

Parameter	Parameter	SI	${f Additional}$
symbol	name	unit	information
q	Heat flux	$\left[\frac{W}{m^2}\right]$	
T	Temperature function	[K]	
∇T	Temperature gradient	$\left[\frac{K}{m}\right]$	
k	Material thermal conductivity	$\left[\frac{W}{m \cdot K}\right]$	
c_{vs}	Volume specific heat capacity	$\left[\frac{J}{kg\cdot K}\right]$	
x	Location	[-]	Vector of coordinates
t	Time	[s]	$t \in \mathbb{R}_+ \cup \{0\}$

Table 1. Symbols used in equations 1 and 2.

Both of described equations have initiated the classical heat transfer theory. However, the mentioned approach is not correct for modern nanoelectronic structures [3] due to the fact that some unrealistic behaviours are assumed. One of them postulates that the heat can propagate instantaneously. The other one indicates that the temperature gradient as well as the heat flux can change their values immediately without any time delays. These examples show that the classical Fourier theory cannot be applied for modelling of the temperature distribution in nanosized structures because of the research results presented in [4], [5], [6], [7]. T. Raszkowski, A. Samson and Mariusz Zubert

Due to this fact, other thermal models appropriate for temperature distribution modelling is submicron structures are needed. One of them, called the Dual-Phase-Lag model, will be presented in the next chapter. Moreover, the detailed problem description will be presented. After that, the simulations and their main results will be demonstrated and carefully discussed. Finally, the conclusion will be added.

2. Methodology

This section contains the detailed description of the chosen thermal model and the characterization of the structure which will be investigated.

2.1. Thermal Model Description

As it was mentioned previously the classical Fourier-Kirchhoff approach cannot be used for modelling the heat conduction in modern nanoelectronic devices. Thus, some modifications of this classical model had to be done. One of the most valuable solutions has been proposed by Tzou at the end of the twentieth century. Tzou has established the Dual-Phase-Lag heat transfer model which includes the significant improvements in relation to the classic Fourier theory.

$$\frac{-1}{c_{vs}}\nabla q\left(x,t\right) = \frac{\partial T\left(x,t\right)}{\partial t} \tag{3}$$

$$k\tau_T \frac{\partial}{\partial t} \nabla T\left(x,t\right) + k\nabla T\left(x,t\right) + \tau_q \frac{\partial q\left(x,t\right)}{\partial t} = -q\left(x,t\right) \tag{4}$$

As it can be seen, the equation (3) is similar to formula (2) because it is based on the Fourier-Kirchhoff equation. On the other hand the most significant modification is shown in equation (4). The Table 2 presents the explanations of symbols used in analysed expression.

Parameter	Parameter	SI	Additional	
\mathbf{symbol}	name	\mathbf{unit}	information	
$ au_T$	Temperature time lag	[s]	$\tau_T \in \mathbb{R}_+ \cup \{0\}$	
$ au_q$	Heat flux time lag	[s]	$\tau_q \in \mathbb{R}_+ \cup \{0\}$	

Table 2. Symbols used in Dual-Phase-Lag equation.

It is worth highlighting that the name of described model comes from the existence of two time lags which description is presented in Table 2.

The mentioned Dual-Phase-Lag model has been chosen to obtain the temperature distribution in the nanosized structures due to the fact that it is characterized by several properties which are adequate for the problem that will be considered in this paper. First of them is related to the fact that Dual-Phase-Lag model is a good approach for both the thermal problems which can be described by hyperbolic equations as well as heat transfer problems based on parabolic equation such as the Fourier-Kirchhoff equation. The second valuable property of the Dual-Phase-Lag model is ability to use it for very small structures and integrated circuit which frequency of the operation is very high [3].

2.2. Structure Description

The analyzed structure has three main layers and contains two nanosized platinum resistors. The first layer, placed at the bottom part of the structure, has 400 m of width and is made of the silicon. The second layer, placed at the middle part of the analyzed structure, has 500 nm of width and it is is made of the silicon nitride or the silicon dioxide. The third layer, placed at the top part of the structure, has 100 nm of width and is also made of silicon nitride or silicon dioxide. The mentioned layer contains the platinum resistors. Each resistor has 100 nm of length and 50 nm of width. The distance between analyzed resistors is equal to 100 nm. The length of the entire structure is equal to 2 mm while its width equals 400.6 m. The cross-section view of the investigated structure is demonstrated in Fig. 1. The description of all parameters presented in Fig. 1 is shown in Table 3.



Fig. 1. The cross-sectional view of the analyzed structure.

Parameter	Parameter	Parameter
\mathbf{symbol}	$\mathbf{value}\left[\mathbf{m} ight]$	Description
S_{H_L}	ca. 0.001	Length of the part between the
		heater and the structure edge
S_{T_L}	ca. 0.001	Length of the part between the
		thermometer and the structure
		edge
T_W	0.0000001	Structure top layer width
M_W	0.0000005	Structure middle layer width
B_W	0.0004	Structure bottom layer width
R_{T_L}	0.0000001	Length of the thermometer
R_{H_L}	0.0000001	Length of the heater
R_W	0.00000005	Resistor width
R_D	0.0000001	Distance between the thermome-
		ter and the heater
S_L	0.002	Total structure length
S_W	0.0000004006	Total structure width

Table 3. Description of parameters of the analyzed structure.

In order to reduce the time of the simulations and the needed computational power, the square-shaped excerpt of the analyzed structure is considered. The side of the square is equal to 1.1 m. The mentioned excerpt consists of the same layers which have been described in the case of the entire structure. However, the bottom layer has only 500 nm of width. Thicknesses of the remaining layers are the same like previously. Moreover, the length of the structure has been also shrunk. Due to this fact, the length of the part of the structure between the structure edges and the resistors are equal to 400 nm instead of approximately 1 mm. The described excerpt of the structure is presented in the Fig. 2. The descriptions of new dimensions are shown in Table 4.

The remaining part of the structure, which is not considered in the previously described excerpt, is modelled taking into account the Neumann boundary conditions. This simplification allows considering only the thermal resistance because thermal capacitances are neglected. It is the result of the assumption postulating that thermal time constants related to the external part of the structure are considerably greater than time of the thermal analysis.



Fig. 2. The cross-sectional view of the excerpt of the analyzed structure.

Parameter	Parameter	Parameter		
symbol	$\mathbf{value}\left[\mathbf{m} ight]$	Description		
E_L	0.0000011	Structure excerpt total length		
E_{H_L}	0.0000004	Length of part of structure ex-		
		cerpt between structure excerpt		
		edge and the heater		
E_{T_L}	0.0000004	Length of part of structure ex-		
		cerpt between structure excerpt		
		edge and the thermometer		
E_W	0.0000004006	Structure excerpt total width		
E_{T_W}	0.0000001	Width of the structure excerpt		
		top layer		
E_{M_W}	0.0000005	Width of the structure excerpt		
		middle layer		
E_{B_W}	0.0000005	Width of the structure excerpt		
		bottom layer		

Table 4. Description of parameters of analyzed excerpt of the structure.

2.3. Results of the Simulation

The temperature distribution in analyzed structure has been obtained using Fourier-Kirchhoff model as well as Dual-Phase-Lag model. It was assumed that one of the resistors, located on the left side of the structure, has been heated while the second one, located on the right side of the structure, is the thermometer. During the simulation the material parameters values presented in Table 5 have been used. The mentioned table has been prepared based on [8].

Parameter	Parameter	Parameter
symbol	$\mathbf{value}\left[\mathbf{m}\right]$	Description
ρ_{Si}	$2330\left[\frac{kg}{m^3}\right]$	Density of the silicon (Si)
$ ho_{Pt}$	$21450\left[\frac{kg}{m^3}\right]$	Density of the platinum (Pt)
ρ_{SiO_2}	$2220\left[\frac{kg}{m^3}\right]$	Density of the silicon dioxide (SiO_2)
$ ho_{Si_3N_4}$	$2400\left[\frac{kg}{m^3}\right]$	Density of the silicon nitride (Si_3N_4)
$c_{\rho_{Si}}$	$712\left[\frac{K}{kg\cdot K}\right]$	Specific heat capacity of the silicon (Si)
$c_{\rho_{Pt}}$	$133\left[\frac{K}{kg\cdot K}\right]$	Specific heat capacity of the platinum (Pt)
$c_{ ho_{SiO_2}}$	$745\left[\frac{K}{kg\cdot K}\right]$	Specific heat capacity of the silicon dioxide (SiO_2)
$c_{ ho_{Si_3N_4}}$	$691\left[\frac{K}{kg\cdot K}\right]$	Specific heat capacity of the silicon nitride (Si_3N_4)
k_{Si}	$148\left[\frac{W}{m\cdot K}\right]$	Thermal conductivity of the silicon (Si)
k_{Pt}	$71.6\left[\frac{W}{m \cdot K}\right]$	Thermal conductivity of the platinum (Pt)
k _{SiO2}	$1.38 \left[\frac{W}{m \cdot K}\right]$	Thermal conductivity of the silicon dioxide (SiO_2)
k _{Si3N4}	$16\left[\frac{W}{m\cdot K}\right]$	Thermal conductivity of the silicon nitride (Si_3N_4)
α_{Si}	$89.2 \cdot 10^{-6} \left[\frac{m^2}{s}\right]$	Thermal diffusivity of the silicon (Si)
α_{Pt}	$25.1 \cdot 10^{-6} \left[\frac{m^2}{s}\right]$	Thermal diffusivity of the platinum (Pt)
α_{SiO_2}	$0.834 \cdot 10^{-6} \left[\frac{m^2}{s}\right]$	Thermal diffusivity of the silicon dioxide (SiO_2)
$\alpha_{Si_3N_4}$	$9.65 \cdot 10^{-6} \left[\frac{m^2}{s} \right]$	Thermal diffusivity of the silicon nitride (Si_3N_4)

Table 5. Material parameters of the analyzed structure.

The numerical solution has been yielded using FEM method. The discretization mesh has been consisted of over 3500 triangles. It is presented in the Fig. 3.



Fig. 3. Discretization mesh for excerpt of the analyzed structure.

The temperature rises in both investigated resistors are presented in Fig. 4 and Fig. 5.



Fig. 4. Comparison of the temperature rise in the heater.



Fig. 5. Comparison of the temperature rise in the thermometer.

The first of them shows the temperature rise obtained using Fourier-Kirchhoff model while the second one reflects the rise of the temperature received using Dual-Phase-Lag model.

The transient analyses show that the average difference between temperatures observed in both resistors does not exceed 1 K. In the case of the Fourier-Kirchhoff model, the initial temperature rise is significant however, it slows down after few 5 s and it stabilizes after about 15 s. In the case of the Dual-Phase-Lag model, the temperature rises significantly slower than in the Fourier-Kirchhoff case. For example, the 6 K growth in the temperature of the heater is observed after about 2 s in the case of the Fourier-Kirchhoff model and after about 900 s in the case of the Dual-Phase-Lag model. The full comparison of the temperature rises observed both investigated thermal model is presented in Fig. 6.

As it can be seen, the temperature distributions obtained using Fourier-Kirchhoff model as well as Dual-Phase-Lag model have the similar behaviour however the similar temperature changes are observed in different instants. All temperature changes occurred in Dual-Phase-Lag model are delayed in relation to respective changes which are observed in Fourier-Kirchhoff model.



Fig. 6. The temperature rise comparison.

3. Conclusions

This paper shows the numerical solutions of heat transfer problem in nanometric multilayer electronic structure containing nanosized resistors. The mentioned solution has been yielded based on the FEM method. During the simulation two different thermal models have been used. The results received using both of them have been compared. This comparison allows confirming that temperature rises in Fourier-Kirchhoff model occur magnificently faster than that ones obtained using Dual-Phase-Lag model. It indicates that in the case of thermal analyses in such small structures the temperature distribution description based on Dual-Phase-Lag model is significantly more reliable than Fourier-Kirchhoff one.

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MODELOWANIE ROZKŁADU TEMPERATURY W STRUKTURACH NANOELEKTRONICZNYCH PRZY UŻYCIU MODELU DUAL-PHASE-LAG

Streszczenie

W pracy przedstawiono porównanie rozkładu temperatury w nanometrycznej strukturze wielowarstwowej przy użyciu modelu Fouriera-Kirchhoffa oraz Dual-Phase-Lag. Rezultat numeryczny otrzymany został przy użyciu metody FDM. Otrzymane wyniki zostały dokładnie zaprezentowanne oraz opisane. Ponadto, wskazano, który z użytych modeli jest bardziej odpowiedni do modelowania temperatury w przypadku struktur nanometrycznych.

Słowa kluczowe: Dual-Phase-Lag, Fourier-Kirchhoff, przepływ ciepła, równanie przewodnictwa ciepła, nanoelektonika, rozkład temperatury