International Journal of Thermal Sciences 114 (2017) 139–154

Contents lists available at ScienceDirect

International Journal of Thermal Sciences

journal homepage: www.elsevier.com/locate/ijts

Monte-Carlo parallel simulation of phonon transport for 3D silicon nano-devices

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ARTICLE INFO

Article history:
Received 21 May 2016
Received in revised form
18 December 2016
Accepted 18 December 2016

Keywords:
Monte-Carlo
Nanoscale
MOS devices
Phonon transport
Boltzmann equation

ABSTRACT

Due to the importance of the transistors in nano-electronics technology, the accurate study of these nano-devices is an essential field of research. Taking into account the non-Fourier nature of heat transfer with considering the three-dimensional structure of the silicon nano-devices, are the challenges in transistor analysis which have not been studied precisely yet. Using the Monte-Carlo method for solving the Boltzmann equation, two actual three-dimensional silicon transistors are accurately simulated. First, the accuracy of the method is verified by the investigation of heat transport in different regimes for a cuboid. Then, the procedure is used to simulate a 2-D silicon nano-device. The obtained results present good consistency with the existent data. Then, the 3-D silicon structure is investigated in two different cases with various boundary conditions, and the formation of the hot zone is announced. Farther, it is attained that a temperature-jump occurs around the time $t = 22$ *ps*. This phenomena is attributed to the change of the type of the dominant heat carriers from acoustic phonons to the optical ones. Furthermore, it is found that although the transistor is still heated the peak temperature starts to decrease when time passes $t = 200$ *ps*. Moreover, as the heat source is switched off at $t = 500$ *ps*, the temperature is acquired to suffer many fluctuations until the expecting descending behaviour appears at $t = 726$ *ps*. Such deportment takes place due to the imprisoning the existent heat in the hot-spot between the isolated boundaries. Besides, the results reveals that redesigning the transistors in case two by leaving the end parts of the top boundary which are in contact with the metallic material open, strengthens the presence of the hot-spot while fastening the heat release to the environment. Also the temperature profiles of the second case exhibits odd behaviours as well. Finally, it should be emphasized that this research compensates the lack of heat transfer data for the thermal investigation of 3-D MOS devices.

1. Introduction

The MOS field-effect-transistors are the main blocks of the nano-electronic technology. Nowadays, due to the aim toward more compact, faster, and stronger processors, accurate simulation of what occurs in these vital nano-devices is indispensable. Strictly speaking, the real three-dimensional structure of the transistors with the actual thermal and electrical circumstances should be considered [1].

As the size of the electronic devices shrinks, the use of the prevailing methods like the Fourier's law leads to the wrong predictions. This is due to the appearance of the non-Fourier effects for the systems with dimensions below the micrometer [2]. There are several kinds of methods for the study of non-Fourier heat conduction. From one hand, these procedures include atomistic-statistic methods such as molecular dynamics or methods based on the semi-classical Boltzmann transport equation (BTE) for phonons [3,4]. On the other hand it contains macroscopic continuum models like single phase-lag (SPL) [5], dual-phase-lag (DPL) [6–11] or the thermo-mass theory [12]. Macroscopic models are usually phenomenological methods which need verification for the calculation of coefficients. This requirement, makes the mesoscopic methods, the imperative tool for nano-scale transient heat conduction modeling, which provide the requisite data for corroboration the simple continuum techniques. The methods which deal with solving the BTE [13–19] have taken much attention for a long time. As long as phonons can be considered to be particles, or on other words, the quantum wave effects are neglected, the

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http://dx.doi.org/10.1016/j.ijthermalsci.2016.12.014
1290-0729/

Boltzmann transport equation can be used to model the heat conduction phenomenon. There are two techniques for obtaining the numerical solution of the BTE. One is the deterministic approach, and the other is the stochastic Monte-Carlo (MC) [20] method. Stochastic method, which is also the interest of this paper, usually is used to solve the partial differential equations that involve a large number of independent variables.

Peterson [21] was the first who presented the Monte-Carlo procedure for investigation of the phonon transport. In the work by Peterson, the phonon dispersion and the various phonon polarizations were not considered. The studies by Mazumder and Majumdar [22,23] have resolved these failures. The consideration of optical phonon modes on thermal conductivity calculation was suggested by Narumanchi et al. [24] and Wang [25]. Narumanchi and co-workers applied two assumptions while taking into account optical phonons. The group velocity of optical phonons is taken to be zero and also, no distinction is made between transverse optical (TO) and longitudinal optical (LO) modes. Wang resolved the first simplifier assumption. While the second postulation was rectified with contemplation of the role of various optical phonon modes on thermal conductivity by Mittal and Mazumder [26]. Also, Wong et al. [27] were the first who entered the concept of internal heat generation with simple procedure to the MC simulation. Nowadays, it is a usual and correct method to model the electron and phonon transport separately and this modeling is proven to present acceptable results.

As the Monte-Carlo method uses the physics of phonons, such as, phonon dispersion and phonon scatterings in simulation of the phonon transport, it is confirmed qua an accurate and flexible method. Also, the MC method linearly scales with the number of dimensions and can be used to model complex geometries. Despite these advantages, the MC method is computationally expensive and is predisposed to statistical variations. There have been some efforts to overcome these disadvantages like the steady-state approach which was suggested by Randrianalisoa and Bailis [28] to reduce the computational time and memory for calculation of thermal conductivity of thin films. Also, Hadjiconstantinou et al. [29] presented the variance-reduced stochastic particle simulation method for solving the relaxation-time model of the BTE that results in an efficient computational cost. Nonetheless, until now, the use of the Monte-Carlo method has been limited to almost simple geometries.

This stochastic Monte-Carlo method with different procedures has been used to predict the thermal conductivity of silicon nanowires [30,31], model the phonon transport in porous silicon [32,33], and other transistor candidate compounds [34], and simulate the heat generation process in silicon MOSFETs [35–38]. Besides, in contrast to the use of the Monte-Carlo method for two-dimensional nano-devices [39,40]. To the best of our knowledge, the transient heat conduction in 3-D nano-devices is an almost untouched subject of interest [41]. Specifically, there have been no molecular dynamic nor Monte-Carlo investigation of these three-dimensional systems. In the present paper, the Monte-Carlo method is used to study the transient heat conduction in 3-D silicon structure. The concept of heat generation is entered by the method used in Ref. [27]. The heating and cooling procedures are investigated for two different cases of 3-D silicon structures with different boundary conditions. This study fulfills the gap existed in the field of 3-D transient heat conduction modeling, and supports the intransitive data for phenomenological macroscopic calculations.

In this work, in Sec. 2, the geometry and the conditions of the simulated silicon structure are given. The mathematical considerations are presented in Sec. 3. Also, Sec. 4 is involved with the numerical method inspection. Then in Sec. 5, the accuracy of the written three-dimensional code is checked by verification the obtained results with the existent data of a cuboid and a 2-D MOSFET. Finally, the results of the simulation of the 3-D silicon structure with two different boundary conditions are dispensed in 6.

2. Geometry and boundary conditions

The main goal of this paper is performing the non-Fourier Monte-Carlo investigation of the transient heat conduction in SOI three-dimensional silicon structures. Two types of structures with different boundary conditions are investigated. The heat source and boundary conditions are similar to what exists in a real 3-D silicon structure nano-device. As it is seen in Fig. 1(a), the First case is a three-dimensional common silicon nano-device in which the existence of the thick layer of SiO_2 and Si substrates under the silicon channel is presented by the boundary conditions. The front, back, left, right, and top boundaries are assumed to be adiabatic according to the low conductivity of the thick isolating oxide covering the surfaces. The bottom boundary is exposed to the ambient temperature while the temperature jump is taken into account. This boundary condition is named as the open boundary condition. It is assumed that the initial temperature in all parts of the 3-D silicon structure is 299 K.

It is important to note that the most part of the heat generated inside the transistor is conducted toward the bottom and then it is dissipated to the surrounding after passing through the bulk silicon. On the other side, the heat flow through the metallic contacts located on top of transistor cannot supposed to be zero.

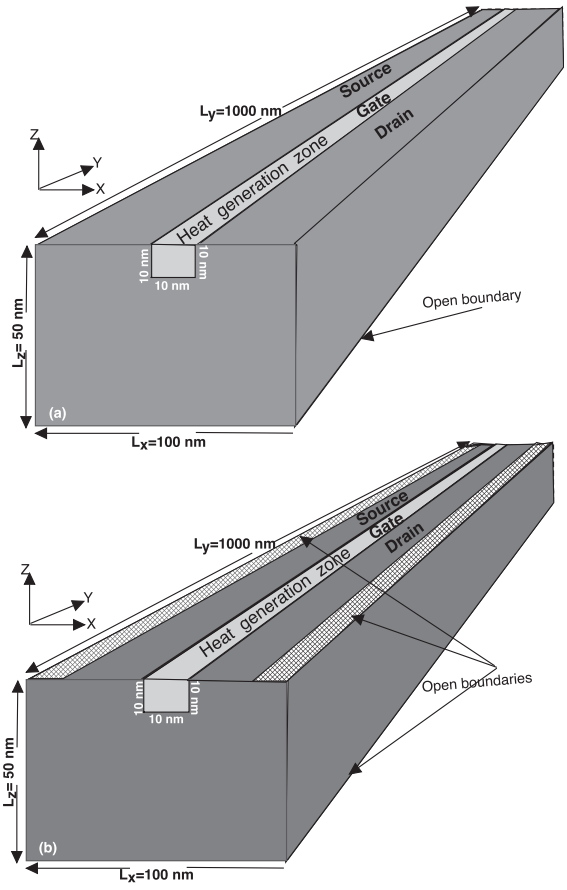

Fig. 1. (a) Case one: the 3-D silicon structure with bottom open boundary condition. (b) Case two: the 3-D transistor with two top and one bottom open boundaries. All other boundaries are adiabatic for both cases.