Monte-Carlo Parallel Simulation of Phonon Transport for 3D Nano-Devices

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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 actual three-dimensional structure of the MOSFETs, 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 MOSFET. The obtained results present good consistency with the existent data. Then, the 3-D MOSFET 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 $t = 22 \text{ ps}$. This phenomena is attributed to the change of the type of

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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 $t = 200 \text{ ps}$. Moreover, as the heat source is switched off at $t = 500 \text{ ps}$, the temperature is acquired to suffer many fluctuations until the expecting descending behaviour appears at $t = 726 \text{ ps}$. 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.

Keywords: Monte-Carlo, Nanoscale, MOS Devices, Phonon Transport, Boltzmann Equation

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. On the other hand it contains macroscopic continuum models like single phase-lag (SPL) [3], dual-phase-lag (DPL) [4, 5, 6] or the thermo-mass theory [7]. 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

20 modeling, which provide the requisite data for corroboration the simple con-
21 tinuum techniques.

22 The methods which deal with solving the BTE [8, 9, 10, 11, 12, 13, 14]
23 have taken much attention for a long time. As long as phonons can be
24 considered to be particles, or on other words, the quantum wave effects are
25 neglected, the Boltzmann transport equation can be used to model the heat
26 conduction phenomenon. There are two techniques for obtaining the numer-
27 ical solution of the BTE. One is the deterministic approach, and the other is
28 the stochastic Monte-Carlo (MC) [15] method. Stochastic method, which is
29 also the interest of this paper, usually is used to solve the partial differential
30 equations that involve a large number of independent variables.

31 Peterson [16] was the first who presented the Monte-Carlo procedure for
32 investigation of the phonon transport. In the work by Peterson, the phonon
33 dispersion and the various phonon polarizations were not considered. The
34 studies by Mazumder and Majumdar [17, 18] have resolved these failures.
35 The consideration of optical phonon modes on thermal conductivity calcu-
36 lation was suggested by Narumanchi *et al.* [19] and Wang [20]. Narumanchi
37 and co-workers applied two assumptions while taking into account optical
38 phonons. The group velocity of optical phonons is taken to be zero and also,

39 no distinction is made between transverse optical (TO) and longitudinal op-
 40 tical (LO) modes. Wang resolved the first simplifier assumption. While the
 41 second postulation was rectified with contemplation of the role of various op-
 42 tical phonon modes on thermal conductivity by Mittal and Mazumder [21].
 43 Also, Wong *et al.* [22] were the first who entered the concept of internal heat
 44 generation with simple procedure to the MC simulation. **Nowadays, it is a**
 45 **usual and correct method to model the electron and phonon trans-**
 46 **port separately and this modeling is proven to present acceptable**
 47 **results.**

48 As the Monte-Carlo method uses the physics of phonons, such as, phonon
 49 dispersion and phonon scatterings in simulation of the phonon transport, it
 50 is confirmed qua an accurate and flexible method. Also, the MC method
 51 linearly scales with the number of dimensions and can be used to model
 52 complex geometries. Despite these advantages, the MC method is compu-
 53 tationally expensive and is predisposed to statistical variations. There have
 54 been some efforts to overcome these disadvantages like the steady-state ap-
 55 proach which was suggested by Randrianalisoa and Bailis [23] to reduce the
 56 computational time and memory for calculation of thermal conductivity of
 57 thin films. Also, Hadjiconstantinou *et al.* [24] presented the variance-reduced

58 stochastic particle simulation method for solving the relaxation-time model
59 of the BTE that results in an efficient computational cost. Nonetheless, until
60 now, the use of the Monte-Carlo method has been limited to almost simple
61 geometries.

62 This stochastic Monte-Carlo method with different procedures has been
63 used to predict the thermal conductivity of silicon nano-wires [25, 26], model
64 the phonon transport in porous silicon [27, 28], and other transistor can-
65 didate compounds [29], and simulate the heat generation process in silicon
66 MOSFETs [30, 31, 32, 33]. Besides, in contrast to the use of the Monte-Carlo
67 method for two-dimensional nano-devices [34, 35].

68 To the best of our knowledge, the transient heat conduction in 3-D nano-
69 devices is an almost untouched subject of interest. Specifically, there have
70 been no molecular dynamic nor Monte-Carlo investigation of these three-
71 dimensional systems. In the present paper, the Monte-Carlo method is used
72 to study the transient heat conduction in 3-D silicon MOSFETs. The concept
73 of heat generation is entered by the method used in Ref. [22]. The heating
74 and cooling procedures are investigated for two different cases of 3-D silicon
75 MOSFETs with different boundary conditions. This study fulfills the gap
76 existed in the field of 3-D transient heat conduction modeling, and supports

77 the intransitive data for phenomenological macroscopic calculations.

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

85 **2. Geometry and boundary conditions**

86 The main goal of this paper is performing the non-Fourier Monte-Carlo
87 investigation of the transient heat conduction in SOI three-dimensional MOS-
88 FETs. Two types of structures with different boundary conditions are inves-
89 tigated. The heat source and boundary conditions are similar to what exists
90 in a real 3-D MOSFET nano-device. As it is seen in Fig. 1(a), the First
91 case is a three-dimensional common MOSFET nano-device in which the ex-
92 istence of the thick layer of SiO_2 and Si substrates under the silicon channel
93 is presented by the boundary conditions. The front, back, left, right, and top
94 boundaries are assumed to be adiabatic according to the low conductivity

95 of the thick isolating oxide covering the surfaces. The bottom boundary is
 96 exposed to the ambient temperature **while the temperature jump is**
 97 **taken into account. This boundary condition is named as the open**
 98 **boundary condition.** It is assumed that the initial temperature in all parts
 99 of the MOSFET is 299 *K*.

100 It is important to note that the most part of the heat generated inside the
 101 transistor is conducted toward the bottom and then it is dissipated to the
 102 surrounding after passing through the bulk silicon. On the other side, the
 103 heat flow through the metallic contacts located on top of transistor cannot
 104 supposed to be zero. Consequently, the conditions of the second sample
 105 is the same as that of case one, with the difference that the two metallic
 106 ending parts of the top surface are also exposed to the ambient temperature.
 107 **This is an accurate consideration as the metallic contacts are the**
 108 **excellent heat conductors.** This open boundary condition helps to more
 109 realizing of the modeling. The sizes of the transistors in our simulation
 110 are $L_x = 100 \text{ nm}$, $L_y = 1 \text{ }\mu\text{m}$, and $L_z = 50 \text{ nm}$, respectively, in *X*, *Y*,
 111 and *Z* directions with the heat generation area of $10 \text{ nm} \times 1 \text{ }\mu\text{m} \times 10 \text{ nm}$
 112 [36]. **It should be noted that only below $t = 50 \text{ ps}$, the geometry**
 113 **can be considered as a 2-D transistor since $1 \text{ }\mu\text{m}$ in the third length**

114 **direction is much longer than the phonon traveling length 30 nm in**
 115 **10 ps.** In the work by Sverdrup and Goodson [37], the heat generation rate
 116 caused by strong electron-phonon scattering is calculated via the electrical
 117 simulation in MEDICI. As the heat generation is peaked on the drain side
 118 of the transistor [37], the region of heat generation is also confined to this
 119 zone heading to a localized heat source. Consequently, to keep away from
 120 electro-thermal coupling, the heat generation rate is modeled with the non-
 121 uniform heat generation profile of $Q_{max}(X + Z - 1)$ accompanied by $Q_{max} =$
 122 $10^{19}W/m^3$. This heat flux is applied for all values of y-coordinate [38].

123 **3. Mathematical modeling**

124 Phonons are the main heat carriers in silicon. As the characteristic length
 125 and the time scale are, respectively, larger than the phonon coherence length
 126 and longer than the phonon relaxation time, the phonons can be treated
 127 as semiclassical particles. Hence, the Boltzmann transport equation is used
 128 to govern these phonons via describing the phonon distribution function,
 129 $f_b(\mathbf{r}, \mathbf{q}, t)$. This distribution depends on the location $\mathbf{r}$, the wave vector $\mathbf{q}$,
 130 and the time t for each phonon branch, b . The phonon Boltzmann transport
 131 equation which includes both equilibrium and non-equilibrium phenomena is

Figure 1: (a) Case one: the 3-D silicon MOSFET 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.

132 written as

$$\frac{\partial f_b(\mathbf{r}, \mathbf{q}, t)}{\partial t} + v_{b,\mathbf{q}} \cdot \nabla_{\mathbf{r}} f_b(\mathbf{r}, \mathbf{q}, t) = \frac{\partial f_b(\mathbf{r}, \mathbf{q}, t)}{\partial t} \Big|_{scat} . \quad (1)$$

133 In equation 1, $v_{b,\mathbf{q}} = \frac{d\omega_{b,\mathbf{q}}}{dq}$ is the group velocity of phonons where $\omega_{b,\mathbf{q}}$ is
134 the angular frequency of branch b with the wave vector $\mathbf{q}$. In general, the
135 frequency depends on both the value and the direction of the wave-vector.
136 With isotropic assumption, the frequency only reliance on the value of the
137 wave-vector and remains same for all directions of the space. In this paper,
138 each phonon branch is treated with the isotropic approximation. Hence,
139 the phonon dispersion relation of the silicon MOSFET will be considered
140 isotropic. Here, the stochastic phonon Monte-Carlo method is used to solve
141 the PBTE. Modeling with the PMC starts with considering the equilibrium
142 condition. The phonon distribution function at the absolute temperature T ,
143 in the equilibrium situation is the famous Bose-Einstein (BE) distribution,
144 $\langle f_{BE} \rangle$ [39].

145 In the MC method, phonons considered as statistical samples are assigned
146 to six individual stochastic spaces: three wave vector and three position vec-
147 tor components. The sampled phonons first undergo drift (ballistic motion)

148 and then, are submitted to the scattering processes. The steps of MC method
 149 for simulating the 3-D silicon MOSFET come in the following section.

150 3.1. Number of Stochastic Samples

151 First, the number of phonons per unit volume that are present in the com-
 152 putational domain, N_{actual} , should be calculated. In the work by Mazumder
 153 and Majumdar [17], the Bose-Einstein density function is measured from
 154 0 K. So, as an instance, in a computational space in which the minimum
 155 available temperature is 300 K, there are many phonons that are not involved
 156 in the heat transfer process, but they only exist to convey the temperature to
 157 300 K. This large amount of phonons takes too much memory and makes the
 158 computation needlessly complex. In the present research, in the continuance
 159 of the work by Wong *et al.* [22], a reference temperature, T_{ref} , which is the
 160 minimum temperature in the solution domain is introduced. Consequently,
 161 as the initial temperature of the sample is taken equal to the reference tem-
 162 perature, the real number of the phonons is zero in the initial condition.
 163 Hence, the actual number of phonons is computed as,

$$N_{actual} = \sum_p \int [f_{BE}(\omega, T) - f_{BE}(\omega, T_{ref})] \frac{|\mathbf{K}|^2}{2\pi^2}$$

$$\frac{d|\mathbf{K}|}{d\omega}|_{\omega}d\omega. \quad (2)$$

Here, $\frac{|\mathbf{K}|^2}{2\pi^2} \frac{d|\mathbf{K}|}{d\omega}|_{\omega}$ or $D(\omega)$ is the phonon density of states. The integration is down over the whole frequency space for each phonon polarization. The integration is numerically performed by discretizing the frequency space. The maximum frequency in each branch, ω_{max} , is driven from each dispersion curve. The frequency interval between 0 and ω_{max} are divided into the N_b intervals with $\omega_{c,i} = \frac{2i-1}{2}\Delta\omega_i$ and $\Delta\omega_i$ being the central frequency and the bandwidth of the i -th spectral bin, respectively. This reduces the integral into a summation over discrete frequency intervals,

$$N_{actual} = \sum_p \sum_{i=1}^{N_b} [f_{BE}(\omega_{c,i}, T) - f_{BE}(\omega_{c,i}, T_{ref})] \frac{|\mathbf{K}|^2}{2\pi^2} \frac{d|\mathbf{K}|}{d\omega}|_{\omega_{c,i}} \Delta\omega_i. \quad (3)$$

In this paper, $\Delta\omega_i$ is taken to be 10^{11} and N_b is 1000. It is shown that for a 3-D silicon, these values of parameters guarantee the accurateness of the solutions. The actual number of phonons obtained from Eq. 3 is usually a very large number which makes the modeling to be computationally expensive. Hence, by introducing the scaling or a weighting factor, W , the number

177 of phonons which are simulated, are decreased:

$$W = \frac{N_{actual}}{N_{prescribed}} \quad (4)$$

178 $N_{prescribed}$ is the number of phonons (stochastic samples) actually initial-
 179 ized/emitted into the system. A same weighting factor, W , is used for each
 180 branch.

181 *3.2. Initialization of Phonon Samples*

182 *3.2.1. Position*

183 The simulation domain is a three-dimensional silicon cube of width L_x ,
 184 length L_y , and height L_z . The sample phonons are spatially initialized by
 185 dividing the computational domain into a number of cells or control volumes.
 186 In 3-D simulations, the control volume is usually taken to be a cube. Hence,
 187 three random numbers, R_1 , R_2 and R_3 , satisfying $0 < R_1, R_2, R_3 < 1$, are
 188 sufficient to determine the coordinates of the phonon ensembles inside the
 189 control volumes. the position vector is obtained as

$$\vec{r} = R_1 L_x \hat{x} + R_2 L_y \hat{y} + R_3 L_z \hat{z} \quad (5)$$

190 Just, initializing the position of the phonon, the frequency should be sampled.

191 The next subsection involves with determining the frequency.

192 3.2.2. Frequency

193 The frequency of the phonon ensembles are sampled by calculating the
 194 number of phonons in the i-th interval of frequency, ω_i . With due attention
 195 to the Eq. 3, the number of phonons in the i-th spectral frequency bin can
 196 be written as:

$$N_i = \sum_p \left(\frac{1}{\exp(\frac{\hbar\omega_{c,i}}{k_B T}) - 1} - \frac{1}{\exp(\frac{\hbar\omega_{c,i}}{k_B T_{ref}}) - 1} \right) \frac{|\mathbf{K}|^2 d|\mathbf{K}|}{2\pi^2 d\omega} \Big|_{\omega_{c,i}} \Delta\omega_i. \quad (6)$$

197 Consequently, a normalized frequency cumulative density function, *CDF* is
 198 constructed,

$$F_i = \frac{\sum_{j=1}^i N_j}{\sum_{j=1}^{N_b} N_j}. \quad (7)$$

199 Here, F_i shows the probability of finding a phonon with frequency less than
 200 $\omega_{c,i} + \Delta\omega_i$. As a result, $F_i - F_{i-1}$ is the probability of finding a phonon in the
 201 i-th frequency interval. For sampling the frequency of the phonon, a random
 202 number R_F , between zero and one, is drawn. Then by using the bisection
 203 algorithm, the i-th frequency bin in which the relation $F_{i-1} < R_F < F_i$ is
 204 satisfied, will be calculated. So, the initial sampled frequency is determined

205 via

$$\omega = \omega_{c,i} + (2R_F - 1)\frac{\Delta\omega_i}{2}. \quad (8)$$

206 *3.2.3. Polarization*

207 After a frequency is assigned to the sampled phonon ensemble, another
208 random number must be introduced to select a polarization, p , or the branch
209 b . The probability of belonging the frequency to the polarization p , in the
210 i -th spectral frequency bin is given by

$$P_{i,p} = \frac{N_{i,p}}{N_i} + P_{i,p-1} \quad (9)$$

211 where, $N_{i,p} = f_0(\omega_{c,i}, p)D(\omega_{c,i}, p)$ is the number of phonons in branch b num-
212 bered by p in the i -th frequency interval. Also, N_i is the total number of
213 phonons in the i -th spectral frequency bin corresponding to the all branches.
214 It should be mentioned that the **transverse modes are degenerate and**
215 **themselves have two branches**. It means there are two TA and TO
216 branches. For example the probability of the existence of the LA phonon in
217 the i -th spectral interval can be calculated as[40, 17]:

$$P_i(LA) = f_0(\omega_{c,i}, LA)D(\omega_{c,i}, LA) \frac{1}{f_0(\omega_{c,i}, LA)D(\omega_{c,i}, LA) + 2f_0(\omega_{c,i}, TA)D(\omega_{c,i}, TA)} \cdots$$

$$\frac{1}{+f_0(\omega_{c,i}, LO)D(\omega_{c,i}, LO) + 2f_0(\omega_{c,i}, TO)D(\omega_{c,i}, TO)}.$$

218 As the probability of the polarization p is calculated, a random number,
 219 R_p is taken into account. If the relation $P_{i-1} < R_p < P_i$ is established,
 220 then the phonon in frequency interval i is ascribed to the polarization p or
 221 branch b . With $p = 1, 2, \dots$ representing different b branches of the dispersion
 222 relation and assuming $P_{i,0} = 0$, the procedure explained is quite general.
 223 In the present work, two acoustic and two optical branches of silicon are
 224 considered. The branches of the sampled phonons frequency are classified
 225 as, LA , TA , LO and TO respectively, for the conditions $R_P < P(LA)$,
 226 $P(LA) < R_P < P(TA)$, $P(TA) < R_P < P(LO)$, and $R_P > P(LO)$.

227 These inputs of the Boltzmann equation are obtained for the present 3-D
 228 silicon MOSFET and is represented in Appendix 8. The calculated actual
 229 number of the phonons, the phonon distribution in frequency space at 300 K ,
 230 and the cumulative density of function F , for the present study are presented
 231 in Figs. 18(a-c) of Appendix. Also, the probability of finding the phonon

232 in each of the branches is shown in Fig. 18(d). Once the frequency and
 233 polarization of the phonon are obtained, the value of its group velocity is
 234 calculated via $v_g = \nabla_k \omega$. The Fig. 19 shows the acquired group velocity for
 235 all branches. In the last step of initialization, the direction is attributed to
 236 the each phonon sample, the procedure is the same as the one described in
 237 [40].

238 3.3. Phonon dispersion

239 The phonon dispersion curves present the relation between the angular
 240 frequency ω and the wave vector q in the first Brillouin Zone (1BZ). These
 241 curves reflect the symmetry of the underlying lattice. From dispersion, the
 242 properties such as group velocity, and density of states can be extracted and
 243 used in the solution of the BTE. Here, isotropic relationships is used to ap-
 244 proximate the dispersion. Silicon has four phonon polarizations **that are**
 245 **two degenerate** acoustic branches named as transverse acoustic (TA) and
 246 longitudinal acoustic (LA). Also there are two optical branches: transverse
 247 optical (TO) and longitudinal optical (LO). The previous studies have con-
 248 firmed that the contribution from optical branches is notable and should be
 249 accounted along the acoustic branches [19, 21].

250 Here, **as the same as done in [41], the quadratic fitting of the**

251 **full dispersion in the (100) crystal direction of the silicon is used**
 252 **to obtain** an approximate isotropic relation for the dispersion of the each
 253 acoustic and optical branches. Hence, the relation $\omega_b = c_b k^2 + v_b k + \omega_{0,b}$ with
 254 $c_{LA} = -2.00 \times 10^{-7}$, $c_{TA} = -2.26 \times 10^{-7}$, $c_{LO} = -1.6 \times 10^{-7}$, and $c_{TO} = 1.12$
 255 in $(m^2/s) \times 10^{-7}$ and the coefficients $v_{LA} = 9.01 \times 10^3$, $v_{TA} = 5.23 \times 10^3$,
 256 $v_{LO} = 0.00$ and $v_{TO} = -2.57 \times 10^3$ in m/s , is applied. Further, the value of
 257 $\omega_{0,b}$ is 0.00, 0.00, 9.88×10^{13} , and 10.2×10^{13} in rad/s , respectively, for the
 258 branches LA , TA , LO , and TO [41].

259 3.4. Phonon drift

260 After establishing the initialized phonons, they are allowed to move from
 261 one point to another. During this transport, the phonons may experience im-
 262 pacts with other phonons, or scattering from boundaries. In MC technique,
 263 the drift and scattering events are treated independently and subsequently.
 264 From mathematical point of view, this means that the transport and scat-
 265 tering parts of the BTE are discontiguous. **In other words the BTE is**
 266 **decoupled in each time step into two equations: the collisionless**
 267 **equation, eq. 10, and the spatially homogeneous Boltzmann equa-**
 268 **tion, eq. 11. The solution of the eq. 10 is used as the initial value**
 269 **for the second step where the eq. 11 is solved [42]. This operator**

270 separation introduces an error which is first-order in time.

$$\frac{\partial f}{\partial t} + \mathbf{v}_g \cdot \nabla \mathbf{f} = \mathbf{0} \quad (10)$$

271

$$\frac{\partial f}{\partial t} = \left[\frac{\partial f}{\partial t} \right]_{scatter} = \frac{f - f_0}{\tau}. \quad (11)$$

272 The position of the phonons that drift inside the 3-D silicon MOSFET
 273 can be traced via using an explicit first order time integration,

$$\mathbf{r}(\mathbf{t} + \Delta \mathbf{t}) = \mathbf{r}(\mathbf{t}) + \mathbf{v}_g \Delta \mathbf{t}. \quad (12)$$

274 In the above relation, Δt is the time step. As the phonons drift, their
 275 frequency range may move from one frequency interval to the other one.
 276 **Hence, according to the new position vector the new spatial bin to**
 277 **which the phonon belongs must be determined.** So, the drift results
 278 in redistribution of energy (and temperature) in the computational domain
 279 [42]. At the end of each drift, the energy of all the phonon ensembles of
 280 each cell are summed, and consequently the energy of each spatial frequency
 281 interval per unit volume, $\tilde{U}_{cell}$, is calculated. Then, the pseudo-temperature
 282 $\tilde{T}$ of each cell, which has no physical meaning, but is introduced for the sake

283 of simplifying the calculation of the scattering processes, can be calculated
 284 by using the Newton-Raphson inversion method,

$$\tilde{U}_{cell}.W = \sum_p \sum_{i=1}^{N_b} \hbar\omega_{c,i} \left[\exp\left(\frac{\hbar\omega_{c,i}}{k_B\tilde{T}}\right) - \exp\left(\frac{\hbar\omega_{c,i}}{k_B\tilde{T}_{ref}}\right) \right]^{-1} \frac{|\mathbf{K}|^2}{2\pi^2} \frac{d|\mathbf{K}|}{d\omega} \Big|_{\omega_{c,i}} \Delta\omega_i. \quad (13)$$

285 Here, $\tilde{T}$ is calculated by considering the presence of thermodynamic equi-
 286 librium within each frequency interval. The phonon may also hit the bound-
 287 aries of the system during the drift. In the next section, these collisions
 288 as an important part of heat transport modeling in nano-scale devices for
 289 determining the change in position and location, will be discussed .

290 3.5. Interaction with the boundaries

291 Considering the free flow, the phonons which are moving in the
 292 space may hit the boundaries. Hence, it is necessary to follow
 293 the trend of the phonons to find out the boundaries at which the
 294 collision has taken place. In this subsection, an algorithm is given
 295 to check the circumstance under which each phonon could possibly
 296 hit the boundaries. In Fig. 2, the schematic of the the phonon
 297 movement is presented. In this figure, O is the origin and the

Figure 2: Phonon hitting the boundary in the three-dimensional space.

vector $\mathbf{OP}$ manifests the initial position of the phonon before the
 free drift. The desired phonon travels along the vector $\hat{s}$. Two sides
 of the following relation display the next position of the phonon,
 the vector $\mathbf{OI}$ [43, 40]:

$$\mathbf{OI} = \mathbf{OP} + \epsilon \hat{s} = \mathbf{OA} + \mu \mathbf{AB} + \nu \mathbf{AC}. \quad (14)$$

If the conditions $0 \leq \mu, \nu \leq 1$, $\epsilon \geq 0$, and $\epsilon \leq v_g \times \Delta t$ are fulfilled, the
 point I is placed in the boundary plane. The mentioned conditions
 should be checked for all boundaries of the computational domain.
 As the values of ϵ and μ are calculated, the point of the intersection of the
 phonon with the boundary is found as

$$\mathbf{OI} = \mathbf{OP} + \epsilon \hat{\mathbf{s}}. \quad (15)$$

307 Next, the behaviour of the phonon ensemble after the collision should be
 308 investigated. A phonon that hit the boundary can be reflected specularly or
 309 diffusively. In specular reflection the phonon with incident direction vector
 310 of $\hat{\mathbf{s}}_i$ undergoes a mirror-like reflection. Hence, the direction vector of the
 311 reflected phonon, $\hat{\mathbf{s}}_r$ will be

$$\hat{\mathbf{s}}_r = \hat{\mathbf{s}}_i + 2|\hat{\mathbf{s}}_i \cdot \hat{\mathbf{n}}|\hat{\mathbf{n}}. \quad (16)$$

312 Here, $\hat{\mathbf{n}}$ is the direction of the outward normal vector of the boundary. In
 313 real boundaries, the reflections are partially specular, and are distinguished
 314 by the value of specularity, α . This factor has the value between zero (for
 315 completely diffusive) and one (for completely specular) reflections.

316 As a phonon ensemble hits a reflective boundary, a random number is
 317 taken into account. If the value of the random number is less than the value
 318 of specularity, the phonon is reflected specularly, otherwise, the reflection is
 319 diffusive. When the phonon undergoes the diffusive reflection, its velocity

direction should be re-sampled as

$$\hat{s} = \sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z}. \quad (17)$$

The degree of specularity varies for the 2-D and 3-D silicon materials. This is due to the difference between the number of diffusive boundaries of these cases. In the present paper, the dimension of the silicon MOSFET is 100 nm, 1 μ m, and 50 nm in X , Y , and Z directions, respectively. Hence, the value of specularity is taken to be equal to 0.885, 0.98, and 0.2228, subsequently, for lateral planes parallel to the XY , XZ , and YZ planes **such that the predicted value of thermal conductivity matches the experimental data.**

3.6. Intrinsic Scattering

A Phonon which travels in a solid can be scattered by means of lattice imperfections (i.e., vacancies, dislocations, and impurities), interactions with electrons, interactions with other phonons (intrinsic scattering), and boundaries. Each of these scattering, which itself can be elastic (means both energy and momentum are conserved) or inelastic (only energy is conserved), result in exchanging energy between different lattice wave vectors.

336 Here, as the 3-D silicon MOSFET is assumed to be pure and perfect,
 337 the scattering due to the vacancies, dislocations and impurities is neglected.
 338 Three-phonon (Umklapp and normal) scattering, and scattering from bound-
 339 aries are the mechanisms, which are considered in the present Monte-Carlo
 340 study of the silicon transistors.

341 Phonon-phonon scattering is the most important mechanism in the usual
 342 temperature range of interest ($300 - 600\text{ K}$) for a silicon MOSFET. Three-
 343 phonon processes can be a normal (N) processes conserving both energy and
 344 momentum or an Umklapp (U) processes, which preserves the energy, but
 345 only conserves the momentum up to a reciprocal lattice vector. Hence, U
 346 processes are the cause for the thermal resistance, while the N processes can-
 347 not be neglected. At low temperatures, they involve in creation of sufficient
 348 number of high-K phonons that participate in U scattering. Therefore, it
 349 is essential to consider the contribution of both N and U processes for the
 350 calculation of the overall relaxation time, scattering rate. Here, like the pre-
 351 vious works, the three phonon interactions are treated through a scattering
 352 rate [17].

$$\tau_{NU}^{-1} = B_L \omega^2 T^3 (LA, Normal + Umklapp) \quad (18)$$

353 and

$$\tau_{NU}^{-1} = B_{TN}\omega T^4 (TA, Normal). \quad (19)$$

354 B_L and B_{TN} are 2×10^{-24} and $9.3 \times 10^{-13} deg^{-3}$.

355 Also, there are some three-phonon Umklapp scatterings which are impor-
 356 tant. The phonon relaxation time in these procedures is calculated via the
 357 Narumanchi suggestion [19] in absence of the optical phonons as

$$\frac{1}{\tau_{i,j}} \approx \frac{\chi\gamma^2}{3\pi\rho v_{ph}^2|\mathbf{v}_g|} \omega_i \omega_{tr} \omega_j r_c^2 \left[\frac{1}{\exp(\hbar\omega_{tr}/k_B T) - 1} - \frac{1}{\exp(\hbar\omega_j/k_B T) - 1} \right], \quad (20)$$

358 Here, v_{ph} is the phase speed of the input phonon which is the ratio of the
 359 frequency to the wave-vector, and v_g is the output phonon group velocity
 360 that is the derivative of the dispersion relation relative to the wave-number.
 361 Also, ω_j is equal to $\omega_i + \omega_{tr}$, and the Grüneisen parameter, γ_b , which presents
 362 the strength of the scattering, is taken to be 0.59. χ is the degeneracy of the
 363 state at the boundary of the FBZ. **In the equation above, $\omega_{tr} = \omega_O - \omega_i$,**
 364 **and ω_O is the optical phonon frequency.** At last, the value of r_c is
 365 calculated as [19]

$$r_c = \frac{2\pi/a - |\mathbf{K}_i|}{2\sqrt{2}}. \quad (21)$$

366 Further, for the mechanism that the optical phonons are also taken part
 367 the scattering rate is calculated as

$$\frac{1}{\tau_{i,j}} \approx \frac{\chi\gamma^2}{3\pi\rho v_{ph}^2|\mathbf{v}_g|} \omega_i \omega_O \omega_{tr}^3 \left[\frac{1}{\exp(\hbar\omega_{tr}/k_B T) - 1} - \frac{1}{\exp(\hbar\omega_O/k_B T) - 1} \right]. \quad (22)$$

368 In this paper, the plots introduced by Henry and Chen for *LO* and *TO*
 369 branches are used to calculate the relaxation times of the optical phonons [44].
 370 The curves are fitted to the mentioned plots for different temperatures in
 371 order to obtain the desired information. It should also be mentioned that
 372 the phonon-phonon scattering with the presence of four or more phonons are
 373 not taken into account. This is due to the fact that this type of scattering
 374 gets important at temperatures much higher than the Debye temperature
 375 which is far from the operating point of most nano-electronic devices. The
 376 obtained results for the relaxation times in different temperatures are given
 377 in Appendix 8.

378 In the Monte-Carlo simulation, the probability of scattering a phonons

379 with the scattering rate of τ_b between time t and $t + \Delta t$ is calculated as,

$$P_{scat} = 1 - \exp\left(\frac{-\Delta t}{\tau}\right). \quad (23)$$

380 Then, a random number R_{scat} is chosen to determine weather the phonon
 381 has been actually scattered. If the probability of scattering, P_{scat} , is greater
 382 than R_{scat} , then the scattering is occurred. When a phonon scatters, its fre-
 383 quency, branch and direction will be re-sampled from the cumulative density
 384 function. Here, the time step, Δt is chosen to be smaller than the minimum
 385 scattering rate of the phonons, which are sampled during the simulation.
 386 Consequently, as the scattering rates are temperature-dependent, the time-
 387 step also relies on temperature. To make sure that the rate of formation of
 388 phonons of a certain state is equal to its rate of destruction, the distribu-
 389 tion function after scattering, F_{scat} , has to be modified by the probability of
 390 scattering:

$$F_{scat}(\tilde{T}) = \frac{\sum_{j=1}^i N_j(\tilde{T}) \times P_{scat,j}}{\sum_{j=1}^{N_b} N_j(\tilde{T}) \times P_{scat,j}} \quad (24)$$

391 As the scattering reestablishes the equilibrium, the outgoing phonon
 392 states are re-sampled from an equilibrium distribution. By using F_{scat} to
 393 re-sample phonon frequency, the energy is kept to be constant during the

394 MC simulation. The rigorous implementation of momentum conservation is,
395 however, harder to address. Since the MC process treats phonons one by
396 one, N or U interactions cannot be rigorously treated.

397 There is also a challenge in re-sampling the phonons after scattering. Only
398 Umklapp processes take part into the thermal resistance. On the other hand,
399 the MC method treats phonons one by one. As changing the direction of the
400 phonons is involved with the form of scattering, so only the direction of the
401 phonons which scatter through a U scattering, are randomly re-initialized.
402 In this study, similar to the work by Lacroix *et al* [26], half of the scattered
403 phonons are re-sampled for their directions. After modeling the scattering
404 process, the energy within each spatial frequency bin is summed up, and
405 local equilibrium temperature is calculated for each spatial bin. Then it is
406 proceeded to the next time step.

407 3.7. Heat generation modeling

408 In the cube of $10 \times 10 \times 1000 \text{ nm}^3$, located in the center of the silicon
409 MOSFET, the heat is generated due to the electric current transport. Hence,
410 this heat generation should be included in the Boltzmann equation. This
411 term is modeled as a resource which heats the region by releasing the phonons
412 into it. In order to prescribe the frequency to the released phonons, the

413 temperature in which the phonons frequency are belonged is determined

$$\sum_P \sum_{i=1}^{N_P} \hbar \omega_i (f_0(\omega_i, T_{pseudo}) - f_0(\omega_i, T_{ref})) D(\omega_i, P) \Delta \omega_i = \frac{U_{cell} \times W}{\Delta X \Delta Y \Delta z} + \frac{E_{gen}}{\Delta X \Delta Y \Delta z}. \quad (25)$$

414 In this relation, $E_{gen}(X, Y, Z)$ is the amount of energy which is generated
 415 during the time interval of Δt . Using this equation, the value of the semi-
 416 equilibrium temperature is calculated. Then, by setting this temperature in
 417 the following relation, the phonon is continuously generated until the total
 418 energy of the phonons become equal to the desired heat generation [22].

$$\sum_{i=1}^{N_{gen}} \hbar \omega_i W \approx E_{gen}(X, Y, Z) \quad (26)$$

419 4. Numerical considerations

420 The written code has become parallel using the OpenMP, the time of
 421 calculation has notably decreased. While considering the parallel code, the
 422 problem is encountered in the generation of random numbers. This is due
 423 to the dependency of producing random numbers on one core. On the other
 424 side, in paralleling the code with OpenMP the memory is simultaneously

425 used by the parallel processors. Since, each random number uses the previous
426 random number as a core, the processors can not generate random numbers
427 in parallel. Hence, the use of random number generation algorithm in parallel
428 codes, not only increases the time of computation, but also makes the results
429 wrong. Consequently, the new algorithm for introducing random numbers
430 is written, in which, all the random numbers are created out of the parallel
431 environment, and then are given to the parallel framework. Although the
432 time consuming strategies have been taken into account, but, the Monte-
433 Carlo method is still too much time consuming, and accordingly needs high
434 performance computers. To be more precise, 8 cores with the specifications
435 of $2.8GHz$ and $32GB - RAM$ were put into service.

436 5. Verification

437 In the following sections, the obtained results of the Monte-Carlo simula-
438 tion are presented. First, the success of the verification is reported. Then, the
439 verification of computation is done for a simple cuboid in different conditions
440 and the 2-D silicon MOSFET.

441 5.1. A cuboid in different regimes

442 Conductive heat transfer is carried out in ballistic and diffusive regimes.
443 In this section, the accuracy of the written code is checked for the situations
444 in which one of the mechanisms is dominant in heat conduction through a
445 cuboid.

446 When the temperature is very low and the environment is too small, the
447 heat conduction is undertaken by the ballistic movement. In this limit, the
448 temperature profile is obtained using the Stefan-Boltzmann law. According
449 to this relation, the temperature all around the cuboid body is constant and
450 is equal to $T_{ballistic} = [\frac{T_h^4 + T_c^4}{2}]^{\frac{1}{4}}$. For a cuboid of size $L_x = 4 \times 10^{-7}m$ and
451 $L_y = L_z = 5 \times 10^{-7}m$, the temperature of the cold and hot walls are taken
452 to be 3 K and 11.88 K, respectively. As a consequence, the temperature of
453 the body should be 10 K. Besides, as the heat transfer happens along the X
454 direction, this direction is divided into 40 segments. Fig. 3 (a) displays that
455 the results of the written code and the precise theoretic solution fit almost
456 very well to each other.

457 The next sample is the one, in which, the diffusive transport is the pre-
458 dominant heat conduction mechanism. This situation is achieved at high
459 temperatures and large sizes. In this limit which is the high Knudsen num-

460 ber regime, the temperature distribution is attained using the Fourier's law.
 461 Due to the model, the temperature varies linearly at steady state condi-
 462 tion. The specimen is again a cuboid, but with size of $L_x = 4 \times 10^{-6}m$ and
 463 $L_y = L_z = 5 \times 10^{-7}m$. The temperature of the hotter boundary is $310\ K$,
 464 while the cold boundary is kept at $290\ K$. The Fig. 3 (b), demonstrates
 465 the acquired behaviour of the temperature profile from the transient regime
 466 till it reaches the steady state in X direction. It is obvious that the linear
 467 behaviour of the steady state assures the correctness of the calculations.

468 5.2. A cuboid with uniform heat source

469 Another system of interest is the one involving the heat source term.
 470 As mentioned in section 3.7, the presence of this term in the Monte-Carlo
 471 calculation is declared by injecting phonons into the computational domain
 472 such that the generated energy of the source gets equal to the energy of these
 473 phonons. In this section, the accuracy of this assumption is checked for a sim-
 474 ple cube of $L_x = 4 \times 10^{-6}m$ and $L_y = L_z = 5 \times 10^{-7}m$. The heat generation
 475 is monotonous and equal to $\dot{g} = 2 \times 10^{15} \frac{W}{m^3}$. The temperature profile is ob-
 476 tained using both the precise solution and the Monte-Carlo simulation. The

Figure 3: (a) The solution in ballistic movement limit along X direction. (b) The transient regime in diffusive limit at X direction.

477 theoretical solution is found via solving the following Fourier-based equation:

$$\nabla \cdot (K_T \nabla T) + \ddot{g}^m = 0; \quad K_T = \frac{1.585 \times 10^5}{T^{1.23}} \quad (27)$$

478 which results in a temperature profile of subsequent form along the X -
479 direction,

$$T(x) = \frac{1}{(-6834.45 \times x + \frac{4.6 \times 10^{11}}{317} x^2 + 2.71 \times 10^{-11})^{(\frac{100}{23})}}. \quad (28)$$

480 This solution and the other one calculated from the Monte-Carlo simula-
481 tion of the Boltzmann equation are shown in Fig. 4. Due to the statistical
482 nature of the Monte-Carlo simulation, some noises are appeared in the solu-
483 tion. Although, the reduction of W makes the fluctuation to decrease, but
484 because of the increased computational cost it is not recommended. Another
485 method to obtain the more precise results in steady state is summing up the
486 temperatures acquired from different times and calculating the time average.
487 This method has computational advantageous, and enhances the reliability
488 of the results.

Figure 4: The temperature profile for a cuboid with the heat generation region.

5.3. 2-D silicon MOSFET

To make sure about the accuracy of the written 3-D Monte-Carlo code, the calculations are carried out for the 2-D silicon MOSFET. The results obtained for case I, are compared to those of Refs. [16] and [45]. In similarity to the work done by Pop *et al.* [45], the heat generation zone of $1 \times 10^{19} \text{ (W/m}^3\text{)}$ at the middle top of the 2-D MOSFET is on for the first 10 *ps*. Fig. 5, presents the comparison between the peak temperature rise versus time obtained from the present code and the available data [45] during starting 10 *ps*.

As it is seen, there is a good consistency between the achieved results and those of the previous studies. This reveals the accuracy of the written code and makes it a reliable calculation. Throughout the time of switching

Figure 5: The peak temperature rise relative to time for a 2-D silicon MOSFET transistors.

501 on the heat generation zone, the temperature increases very fast. Figure 6(a)
 502 manifests that turning off the heat source, the MOSFET does not immedi-
 503 ately starts to get cool, and the maximum temperature occurs at $t = 13 \text{ ps}$.
 504 The temperature enhancement after switching off the heat generation zone,
 505 indicates the presence of non-equilibrium heat transfer. In other words, the
 506 accumulation of phonons in a limited region, makes them to be pumped out
 507 with delay. The ballistic movement causes the phonons to diffuse in all di-
 508 rections and such diffusion results in the reduction of heat reaching the heat
 509 exchange boundaries. The temperature contour at $t = 60 \text{ ps}$, is manifested in
 510 Fig. 6(b). It is obtained that it takes 50 ps , five times greater than the heat-
 511 ing time, for the 2-D MOSFET to get almost cool. This finding demonstrates
 512 deficiency in the design of the MOSFETs.

Figure 6: (a) The maximum temperature relative to the time for a 2-D MOSFET during heating-cooling procedure. (b) The temperature contours at $t = 60$ ps.

513 6. Results and Discussions

514 As mentioned, the three-dimensional Monte-Carlo simulation is performed
515 to study the heat transfer in two 3-D silicon MOSFETs with different bound-
516 ary conditions. In case one the heat is only transferred within the bottom
517 boundary, while the second case is also involved with heat emitting from two
518 separate portions of the top boundary in addition to the energy transferred
519 from the underneath. In addition, the heat generation is considered to be
520 inhomogeneous in both transistors.

521 6.1. Case one

522 The case one is investigated in two distinct situations. First, the 3-D
523 MOSFET is affected by the heat source during whole 500 *ps* of computation
524 time. The entire system is initially kept at 299 *K*. The peak temperature
525 versus time-step number is plotted in Fig. 7(a). As it is seen, the peak tem-
526 perature starts to decrease after times greater than 200 *ps*. This finding
527 can be justified by analyzing the input/output energy plots. In Fig. 7(b),
528 **the blue line presents the energy which is exited from the bottom**
529 **boundary of the nano-device into the environment. The black line**
530 **shows the whole input energy that is the summation of the gen-**

531 **erated heat in the gate, violet line, and the income energy from**
 532 **the boundaries, the red line. In more details,** a number of phonons as
 533 a source of heat generation and the input heat are entered to the computa-
 534 tional space. Also, some phonons leave this space from the bottom boundary.
 535 After $t = 200 \text{ ps}$, the trend of the plots reverses, and the output energy be-
 536 comes larger than the input energy. Consequently, the temperature decrease
 537 between 44 ps and 66 ps , is the result of heat egression from the open bound-
 538 ary. In other words, it takes 44 ps for phonons to travel the 50 nm distance
 539 to touch the underneath boundary, and alter the temperature profile. Hence,
 540 the group velocity of this type of phonons is $1022.73 \frac{\text{m}}{\text{s}}$, which determines
 541 that they belong to the optical branches or the TA mode.

542 Further, it is obtained that around $t = 22 \text{ ps}$, a temperature jump of
 543 60 K occurs. This abrupt growth takes place when the peak temperature has
 544 reached the temperature 400 K . The phonons that do not diffuse through the
 545 MOSFET, gather in a small region and make the hot spot. In the present 3-D
 546 transistor, the hot phonons are piled up in a zone with $50 \text{ nm} < X < 70 \text{ nm}$
 547 and $30 \text{ nm} < Z < 50 \text{ nm}$. It is found that before the appearance of the
 548 temperature jump, the acoustic phonons are the prevailing phonons existed
 549 in the hot-spot. As a consequence, due to their larger group velocity relative

Figure 7: (a) The peak temperature rise versus time for a 3-D MOSFET in the presence of the heat zone. (b) **The trend of energy in 3-D MOSFET boundaries. The blue line shows the energy exited from the bottom boundary of the nano-device into the environment. The black line shows the whole input energy that is the summation of the generated heat in the gate violet line, and the income energy from the boundaries, the red line.**

550 to the optical phonons, they carry away the heat from the hot-zone. On
 551 the other side, as time evolves and the jump happens, the number of acous-
 552 tic phonons in the hot-spot region decreases while the amount of optical
 553 phonons grows. **The group velocity of the optical phonons are lower**
 554 **then that of the acoustic phonons, consequently, in a specified pe-**
 555 **riod of time, the amount of the heat carried out of this region by**
 556 **these dominant phonons significantly decreases.** Hence, the reduction
 557 of the heat dissipation arises, which causes this region to experience augmen-
 558 tation of heat energy. The transmutation in the phonon combination towards
 559 the optical phonons with lower group velocity, results in the occurrence of
 560 temperature-jump in the hot spot. Moreover, in a hotter zone, more phonons
 561 with higher frequencies are produced. This leads to the more increment of
 562 the temperature in this region.

563 In the following, the temperature profiles in various XZ , YZ , and XY
 564 planes of the 3-D silicon structure are investigated. The temperature dis-
 565 tribution in XZ plane is manifested for four different times in Figs. 8(a-d).
 566 Figure 8 presents the profile for the time before the abrupt jump in the max-
 567 imum temperature. As it is shown, more than half of the heat energy is
 568 stored in the hot-spot, which is created in the middle top of the MOSFET.

569 This notable energy makes the temperature of this zone to increase.

570 The heat localization in the hot-spot is shown in Fig. 8(b). This figure reveals the temperature profile after the temperature skip. As it is seen 571 from Fig. 8(c), the first thermal wave reaches the bottom open boundary 572 at $t = 49.5 \text{ ps}$. Therefore, the minimum temperature of the 3-D MOS- 573 FET, which belongs to the areas far from the hot-spot, gets larger. Further, 574 Fig. 8(d) presents the temperature profile in $t = 200 \text{ ps}$. At this time, the 575 heat removal from the underneath boundary becomes more than the input 576 energy. Then, the transistor starts to get cool, and the heat energy moves 577 from the heat generation zone to the inner parts to make the MOSFET at- 578 tain the equilibrium state. Finally, the steady-state temperature distribution 579 is demonstrated in Fig. 8(e). 580

581 In addition, to analyze the 3-D heat transfer more precisely, the tempera- 582 ture distribution in other planes is also investigated at $t = 500 \text{ ps}$. Figs. 9(a) 583 and (b) display the temperature contours in YZ plane for two different val- 584 ues of $X = 2$ and 60 nm . Also, the deportment of temperature profiles along 585 the XY plane in various Z , is shown in Figs. 9(c-e). As it is demonstrated 586 in Figs. 9(a) and (b), due to the non-uniform generated heat, the heat flux 587 spread in the places nearer to the top-left boundaries is remarkably less than

Figure 8: (a-e) The temperature distribution in XZ plane averaged over Y direction, respectively at $t = 28, 32, 50, 200$, and 500 ps.

588 that of released through the right area. Besides, the penetration of the heat
 589 into the inner parts of the MOSFET and the increase in the temperature of
 590 the lower parts of the transistor is obvious. In Figs. 9 (c-e), the temperature
 591 profile in XY plane for the bottom, the lowest part of the heat generation
 592 zone, and the top of the MOSFET is displayed. The ballistic movement
 593 creates heat islands in cross sections of the transistors. These islands are
 594 more visible around the heat source owing to the presence of more phonons.
 595 Also, they are more likely to be formed in proximity of the left side of the
 596 MOSFET. This is for the reason that the lower temperature of the left side
 597 of the heat generation zone, causes the production of the phonons with less
 598 energy and larger velocity.

599 It is acquired that at $t = 500 \text{ ps}$, the 16 percent of the energy which
 600 is mostly carried by TO phonons, is still within the heat generation region.
 601 This shows that the equilibrium process has taken place, and the heat is prop-
 602 agated around the MOSFET to reduce the maximum temperature. Hence,
 603 the temperature augmentation occurs in the upper one fifth of the transistor
 604 while the remained four fifth of the MOSFET has lower temperature close to
 605 the initial temperature. Also, it has been presented in Figs. 8(a-d) that the
 606 generated heat is concentrated in a limited zone called as a hot-spot. This

Figure 9: (a) The temperature profile for a 3-D MOSFET in the YZ plane at $X = 60 \text{ nm}$ and in $t = 500 \text{ ps}$ in the presence of the heat zone. (b) The same as (a) but for $X = 2 \text{ nm}$. (c-e) The temperature behaviour in XY plane at $t = 500 \text{ ps}$, respectively, for $Z = 50, 40$, and 2 nm .

607 deficiency makes the lifetime of the transistor to decrease. In this wrongly
608 designed MOSFETs, the heat transfer firstly occurs in the X direction, so
609 the temperature as isotherm waves moves along the Z direction. The heat
610 transfer in the X direction instead of the one in Z , causes the time for tem-
611 perature enhancement to increase. The newly designed 3-D transistors have
612 overcome this failure by disspreading the heat all over the MOSFET.

613 At the next step, the heat source of the mentioned 3-D silicon transistor
614 is terminated at $t = 500 \text{ ps}$, and the system is cooled by the energy exchange
615 with the environment until $t = 1 \text{ ns}$. The computational time of this sim-
616 ulation with mentioned CPU characteristics was 2 days, 13 hours and 29
617 minutes. Figure 10, manifests the behaviour of the peak temperature after
618 switching off the transistor, for the time period of 500 ps or up to the time
619 $t = 1 \text{ ns}$. It is obvious that for the first 220 ps , the temperature suffers many
620 fluctuations until the expecting descending trend appears at $t = 726 \text{ ps}$.

621 In the following, the behaviour of the temperature profile will be an-
622 alyzed in more details. Just as the heat source is turned off, an abrupt
623 temperature reduction becomes evident. This prompt reduction trend lasts
624 for nearly 11 ps and then the drastic fluctuations occur. Again, 60 ps after
625 the disconnection of the source/drain current, the temperature starts to grow

Figure 10: (a) The peak temperature rise versus time for a 3-D MOSFET when the heat source is turned off. (b) **The energy behaviour in 3-D MOSFET boundaries. The blue line shows the energy exited from the bottom boundary of the nano-device into the environment. The black line shows the whole input energy which in the cooling time is equal to the income energy from the boundaries.**

626 unexpectedly. Moreover a temperature jump takes place and then the tem-
 627 perature remains constant for an interval. Finally as previously remarked,
 628 at $t = 236 \text{ ps}$ the temperature experiences the conceivably reductive trend.
 629 Figure 10, also exhibits that 500 ps after switching off the transistor, the
 630 same as the time of heating, the maximum temperature in the MOSFET
 631 is 50 K higher than the temperature of the environment. The inability of
 632 the transistor to be cooled in the same time as the time spent for heating,
 633 along with the creation of the hot-spot are the two main difficulties of the
 634 3-D MOSFETs.

635 In this part, the reason for the occurrence of such deportment is given.
 636 **Two mechanisms are responsible for decreasing the peak temper-**
 637 **ature of the nano-device. The first procedure which is presented**
 638 **by the blue solid line in Fig. 10(b) is exiting the heat from the**
 639 **boundary. The other mechanism is the heat diffusion from the hot**
 640 **zone to the inner parts of the nano-system. The most important**
 641 **time interval is between 500 ps and 744.144 ps in which the MOS-**
 642 **FET is affected under the current disconnection shock. The study**
 643 **of the disappearing of the hot spot and the transformation of the**
 644 **phonons from one branch to another kind of the branch gives accu-**

645 **rate information about the process of cooling the transistor. The**
 646 **mechanism that firstly causes the intense temperature reduction**
 647 **in the device is the heat diffusion inside the device.** Switching off the
 648 heat source, the abrupt temperature decrease presents itself because of the
 649 heat propagation in the transistor. During this mechanism the hot spot zone
 650 destroys while transferring the heat to the other areas of the nano-device.
 651 As a consequence of the presence of five boundaries around the center of the
 652 heat generation zone, the heat distribution along the X direction is somehow
 653 imprisoned, and accordingly the heat transfer is more visible alongside in
 654 comparison to the heat diffused through the Z direction. Although the tem-
 655 perature gradient along the Z direction is almost constant, as it seen in Fig.
 656 11(a), the heat diffusion across the X direction makes the heat propagation
 657 from the hot zone the most effective temperature reducer for a time interval
 658 of 26 ps . After the time $t = 526\ ps$, the heat is nearly distributed along
 659 the X -direction, and the heat transfer through the Z direction decreases the
 660 maximum temperature. Also, the Fig. 11(b) demonstrates the poor heat
 661 propagation along Z until the time $t = 526\ ps$.

662 As the time passes, the two procedure of heat propagation from the
 663 hottest region and the heat exchange with the environment from the bot-

Figure 11: (a) The Y -averaged temperature distribution in the XZ plane at $t = 526$ ps when the heat zone is switched off at $t = 500$ ps. (b) The same as (a) but for $t = 744$ ps. (c) The temperature distribution in YZ plane at $X = 50$ nm when $t = 526$ ps. (d) Alike the (c) but when $t = 744$ ps.

Figure 12: (a) The temperature profile for a 3-D MOSFET in the YZ plane at $X = 50 \text{ nm}$ when $t = 1 \text{ ns}$. (b) The temperature distribution averaged over Y direction in the XZ plane at $t = 1 \text{ ns}$. (c) The temperature behaviour over the XY plane at $Z = 50 \text{ nm}$ and $t = 1 \text{ ns}$.

tom boundary cause the temperature all over the 3-D transistor to lessen.
 nevertheless, as Fig. 11(c) displays at $t = 744 \text{ ps}$, the limited heat energy
 is confined on top of the 3-D MOSFET, and does not evacuate to the other
 places. This heat accumulation in a narrow area on top of transistor, dis-
 penses the critical deficiency in transistor design. Also as the Fig. 11(d)
 suggests the heat propagation along the Z -direction have become faster at
 $t = 744 \text{ ps}$. It is also obtained that the type of the phonon branch is a
 significant parameter in heat transfer behaviour of device. In the cooling
 process of the transistor, the type of the dominant phonons changes from
 the optical branch to the acoustic one. Consequently, the group velocity of
 the phonons increases, and the ballistic behaviour of the heat transfer gets
 stronger. As mentioned, first, the heat diffuses from the center of the hot-spot
 to all around the MOSFET, but then the heat energy in upper parts of the
 transistor imprisons between the five boundaries. Figures. 12(a-c) manifest
 the temperature profiles in XZ , YZ , and XY planes 500 ps after switching
 off the heat source. In order to rectify the deficiencies of the 3-D transistor,
 the second case with improved boundary conditions is investigated.

6.2. Case two

In order to resolve the deficiencies appeared in the case one, the transistor of case 2 is introduced. In this type of transistor, in addition to the heat exchange from the bottom boundary, the open boundary is considered in both sides of the top boundary. The size of the new designed MOSFET is the same as that of the case one. The heat generation is also non-uniformly distributed.

At first, the heat source is switched on for the whole 500 ps time of the simulation. Figure 13(a) presents the peak temperature versus time. Also, the power curve fitted to the obtained data is displayed on Fig. 13(a). The W factor is considered to be 184. The Fig. 13(b) manifests the behaviour of the energy current at the boundaries. As it is seen, the output heat energy is equal to the input energy between the time interval of $t = 22.2 ps$ to $t = 44.4 ps$. Hence, the maximum temperature remains constant during this period of time. After this time, due to the more generated heat relative to the lost energy, the peak temperature arises until $t = 88.8 ps$. Then, ignoring the fluctuations occurred because of the statistical behaviour of the numerical method, and the nature of the ballistic movement, the maximum temperature follows the reduction trend.

Figure 13: (a) The peak temperature rise versus time for a 3-D MOSFET with two top open boundaries and the open bottom boundary through the heating. (b) The energy behaviour of the 3-D MOSFET with new defined advantageous boundary conditions.

700 Reaching the time of $t = 222.2 \text{ ps}$, the heat pumped to the environment
 701 from the top open boundaries and the heat exited from the bottom boundary
 702 get commensurate. As described the area of the top open boundaries are
 703 likely one fifth of that of the bottom boundary. This fact reveals that the
 704 temperature gradient on top of the MOSFET is notably larger than the
 705 temperature slope in the bottom boundary. The temperature profiles in
 706 YZ planes, which are averaged along the X direction for two intervals of
 707 $0 < X < 10 \text{ nm}$ and $90 < X < 100 \text{ nm}$ are respectively manifested in Figs.
 708 14 (a) and (b). This averaging is performed through the places of the top
 709 open boundaries at $t = 200 \text{ ps}$. This figures verify the larger gradient near the
 710 top boundaries specially at the left one. Also, the temperature distributions
 711 on the same positions for $t = 500 \text{ ps}$ are plotted in Figs. 15(a) and (b).
 712 It is clear that the temperature gradient at the bottom boundary has been
 713 increased at $t = 500 \text{ ps}$. Hence, the exited heat from the underneath border
 714 becomes larger than the energy sent out from the top open boundaries.

715 The comparison of the plot demonstrated in the Fig. 7(a) with that of
 716 Fig. 13(a), reveals that the presence of two open boundaries on top of the 3-D
 717 MOSFET strengthens the effect of hot-spot formation. To be more precise,
 718 the value of the maximum temperature of the second case increases more

Figure 14: (a) The temperature profile in YZ plane averaged over the $X = 1$ to 10 nm top open boundary when $t = 200 \text{ ps}$. (b) The temperature distribution across the YZ plane averaged along the $X = 90$ to 100 nm top open boundary.

Figure 15: (a,b) The same as Fig. 13(a,b) but when $t = 500$ ps. (c) The 3D plot of Y-averaged temperature profile in XZ plane at $t = 500$ ps.

719 and faster than the peak temperature appeared in the first geometry. Also,
720 Figs. 13(b) and 7 (b) manifest that although the input energy of the both
721 geometries are the same, the total output energy of the second case grows
722 further and more rapid. The enhancement of hot-spot influence is due to the
723 reduction of the temperature gradient along the Z -direction which itself is
724 the result of the presence of the two open top boundaries. In spite of the fact
725 that the total output heat is larger for case 2, the less gradient makes the
726 energy to concentrate more in a hot-spot, and inevitably less heat reaches
727 the bottom boundary in a longer time.

728 It is obtained that the time effect is more pronounced than the size influ-
729 ence for the second geometry. In other words, the heat concentration in the
730 MOSFET is due to the short time of the heat exchange, and accordingly the
731 important procedure in the heat removal is the heat diffusion in the MOS-
732 FET rather than the heat exchange with the surroundings. It should be
733 added that the amount of heat energy which is trapped in the hot-spot is
734 17.7% of the total energy for the second case, while this percentage for the
735 first geometry is 15.9%. But, as the total energy of the case two is lower than
736 the case one, the heat energy inside the first geometry is lower. In addition,
737 the heat concentration in the hot-spot can be attributed to the presence of

738 less TA phonons due to more scattering.

739 After $t = 500$ *ps*, similar to case 1, the heat source is switched off. Then,
740 the thermal cooling mechanism is studied for the next 500 *ps*. The W factor
741 is taken to be 184. The simulation has been performed for 2 days, 9 hours, 17
742 minutes and 31 seconds to get the result. The obtained peak temperature-
743 rise and the energy current are displayed in Figs. 16 (a) and (b). The
744 comparison between Fig. 16 (a) and Fig. 10 (a) reveals that although the
745 top open boundaries cause more temperature enhancement throughout the
746 heating, but they make the cooling simpler. Once the heat generation is
747 stopped, more heat is transferred through the top boundary which has a
748 larger temperature gradient, and consequently the heat does not accumulate
749 on top of the MOSFET.

750 Fig. 17(a) shows the temperature distribution which is averaged over the
751 Y -direction at $t = 600$ *ps*. It is seen that the maximum temperature which is
752 644.86 *K* at the time when the heat source is turned off, reduces to 387.21 *K*.
753 This shows 40% lessening of the peak temperature when 100 *ps* has been
754 passed. Also, the acquired temperature profile in YZ plan at $X = 50$ *nm*
755 is shown in Fig. 17(b). This figure indicates that the effect of the bottom
756 boundary in heat removal is not significant. Moreover, the behaviour of the

Figure 16: (a) The peak temperature rise versus time for the 3-D silicon transistor when the heating zone is switched off. (b) The energy trend in 3-D silicon transistor in bounding lines.

Figure 17: (a) The temperature profile averaged along the Y -direction in XZ plane. (b) The temperature contour at $X = 50$ nm when $t = 600$ ps in YZ plane. (c) The temperature distribution in XY plane at $Z = 50$ nm and $t = 600$ ps. (d) The 3-D plot of Y -averaged temperature versus X and Z at $t = 1$ ns.

757 temperature in the XY plane is demonstrated in Fig. 17(c) at $Z = 50 \text{ nm}$.
 758 The figure exhibits that the minimum temperature is 320 K , which is 20 K
 759 larger than the environment temperature. Further, it is shown that the
 760 temperature gradient along the X -direction on top of the MOSFET is very
 761 intense such that the heat transmission through this region is prominent.
 762 At last, the temperature distribution in $t = 1 \text{ ns}$ is plotted in XZ plane.
 763 Fig. 17(d) displays this profile. The low temperature difference between
 764 the temperatures of the various places reveals the heat distribution in the
 765 MOSFET.

766 **7. Conclusions**

767 In this paper, the Monte-Carlo simulation of the three dimensional silicon-
 768 based MOSFET is performed. The accuracy of the numerical method is
 769 checked by verifying the obtained results with the existent data. Then, the
 770 3-D MOSFET is studied under two different boundary conditions: (i) only
 771 the bottom boundary exchanges energy with the environment, and (ii) in
 772 addition to the bottom boundary, two top boundaries are also open to the
 773 surrounding. In both cases, the hot zone is formed. For the case one, the
 774 jump in the maximum temperature takes places due to the change in the type

of the predominant heat carriers to the optical phonons. Moreover, many odd behaviours in the temperature profiles are found during the heating and cooling of the 3-D transistor. Also, it is obtained that the efficiency of the 3-D transistors by adding two top open boundaries, is improved. Although the new condition intensify the heat gathered in the hot-spot, it makes the heat spreading to the environment easier. In conclusion, the present work provides the exact data needed for the non-Fourier transient heat transfer analysis of multidimensional MOSFETs.

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8. Appendix

At the first step of solving the Boltzmann equation, the actual number of phonons is obtained. Accordingly, the important parameter W is calculated. This factor should be kept constant during the simulation. The actual number of phonons per volume for different branches in various temperatures are displayed in Fig. 18(a). Moreover, the phonon distribution in

792 miscellaneous frequency intervals is highly non-linear. Hence, a cumulative
 793 density function is needed for ascribing the frequency to the phonon. This
 794 function is introduced in Eq. 7. Fig. 18(b) illustrates the behaviour of the
 795 number of phonons versus frequency. This figure illustrates that the most of
 796 the phonons belong to two main frequencies. The first one which has more
 797 phonons is assigned to the transitional phonons, and the second one is at-
 798 tributed to the optical phonons. Also, as it is seen in Fig. 18(c), using Eq. 7,
 799 and Fig. 18(b) the cumulative density function at different temperatures is
 800 obtained. It is obvious that when the temperature increases, the number of
 801 the optical phonons becomes larger. Besides, different branches are present
 802 in a specific frequency. This affects the type of the predominant phonons in
 803 heat transfer. To be more precise, at low temperatures the TA phonons are
 804 the main heat carriers in the MOSFET, but as the temperature enhances the
 805 presence of this branch fades out while the other kind of phonons appear.
 806 Fig. 18(d) shows the probability of the presence of each type of phonons in
 807 a peculiar frequency.

808 After that, the group velocity of different types of phonons is obtained by
 809 differentiation of the dispersion relations. Fig. 19, represents the comport-
 810 ment of the group velocity as a function of frequency.

Figure 18: (a) The actual number of phonons per volume versus temperature for different branches. (b) The number of phonons as a function of frequency when $T = 300\text{ K}$. (c) The cumulative phonon density of function. (d) The probability of the presence of the phonons in each branch.

Figure 19: The group velocity of the various branches of TA , LA , TO , and LO at $T = 300\text{ K}$.

At last, using the equations introduced in Sec. 3.6, the life-time of the phonons are calculated for different temperatures. As expected, the trend in Figs. 20(a-c) shows that the mean time between the scatterings decreases just when the temperature increases. This reduction is ascribed to the increment of the number of scatterings. Also, the obtained mean free path as an important parameter in the determination of heat transfer regime is shown in Fig. 20(d) when $T = 300\text{ K}$.

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Figure 20: (a) The phonon life-time in different branches at $T = 100$ K. (b) The same as (a) but when $T = 300$ K. (c) The phonon relaxation time in $T = 500$ K. (d) The phonon mean free path for TA, LA, TO and LO branches when $T = 300$ K.

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