Multi Scale Study of Heat Transfer Using Monte Carlo Technique for Phonon Transport

by

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Self-heating degrades the performance of devices in advanced technology nodes. Understanding of self-heating effects is necessary to improve device performance. Heat generation in these devices occurs at nanometer scales but heat transfer is a microscopic phenomena. Hence a multi-scale modeling approach is required to study the self-heating effects. A state of the art Monte Carlo device simulator and the commercially available Giga 3D tool from Silvaco are used in our study to understand the self-heating effects. The Monte Carlo device simulator solves the electrical transport and heat generation for nanometer length scales accurately while the Giga 3D tool solves for thermal transport over micrometer length scales. The approach used is to understand the self-heating effects in a test device structure, composed of a heater and a sensor, fabricated and characterized by IMEC. The heater is the Device Under Test (DUT) and the sensor is used as a probe. Therefore, the heater is biased in the saturation region and the sensor is biased in the sub-threshold regime. Both are planar MOSFETs of gate length equal to 22 nm. The simulated I-V characteristics of the sensor match with the experimental behavior at lower applied drain voltages but differ at higher applied biases. The self-heating model assumes that the heat transport within the device follows Energy Balance model which may not be accurate. To properly study heat transport within the device, a state of the art Monte Carlo device simulator is necessary. In this regard, the Phonon Monte Carlo (PMC) simulator is developed. Phonons are treated as quasi particles that carry heat energy. Like electrons, phonons obey a corresponding Boltzmann Transport Equation (BTE) which can be used to study their transport. The direct solution of the BTE for phonons is possible, but it is difficult to incorporate all scattering mechanisms. In the Monte Carlo based solution method, it is easier to incorporate different relevant scattering
mechanisms. Although the Monte Carlo method is computationally intensive, it provides good insight into the physical nature of the transport problem. Hence Monte Carlo based techniques are used in the present work for studying phonon transport. Monte Carlo simulations require calculating the scattering rates for different scattering processes. In the present work, scattering rates for three phonon interactions are calculated from different approaches presented in the literature. Optical phonons are also included in the transport problem. Finally, the temperature dependence of thermal conductivity for silicon is calculated in the range from 100K to 900K and is compared to available experimental data.
Dedicated to my parents and teachers
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In the recent years, technology has advanced to fabricate integrated circuits (IC) at 14nm gate length commercially[1]. Fab industry giants like Intel, TSMC, Samsung and Global Foundaries have plans to fabricate ICs at 10nm by 2017. Samsung has already fabricated and tested 128Mb SRAM in 10nm[2] and hoping to commercialize the process by end of 2016. This aggressive scaling of technology is possible because of the advent of FinFET, FDSOI technology.

The device miniaturization results in large quantity of heat generated per unit volume[3]. This results in overheating of the device which degrades its performance and reliability of devices. A recent study on self-heating of 14nm to 7nm bulk silicon FinFETs show that heat confinement in Si channel increases by 20% and in strained Ge channel by 57%[4]. This results in 70K and 100K change in channel temperature in 14nm and 7nm FETs. Hence efficient heat removal methods are necessary to increase performance and reliability.

A recent trend in peak efficiency versus power density of the switched capacitor power converters shows that the efficiency decreases as power density increases[5]. This shows the efficiency of utilizing the electrical energy in logic operations is getting reduced as the power density is increasing. This means the thermal energy is getting generated higher and higher with increased power density and is not useful in any operation of the system. New innovations can help to utilize this waste energy rather than to just remove from the system.

The control of electrons in semiconductors has resulted in great technological advancement in computing, signal processing, bio-medical applications etc. The control
of photons in different materials has generated technological revolution in wireless communications, optical fiber applications, microwave applications etc. These applications are significantly helping in all the day to day activities. Another particle similar to electrons and photons is phonon. It is a particle that carries heat energy in the materials. Like electrons and photons, with the control of phonons in materials new innovations are possible[6]. For example acoustic diodes and thermal diodes are the diodes which pass sound and heat in a unidirectional way similar to electronic diode. To understand how these devices operate and propose new innovations with these devices, the phonon transport problem should be studied and understood very well. Hence the study of phonon transport in materials is a necessary step to further advance in technology.

The present work focuses on understanding the heat transport in nanoscale electronic devices. The study is mainly on understanding and modeling the self-heating effects (SHE) of 22nm planar MOSFETs and how the heat transport occurs at die packaging scale. The structure of the 22nm MOSFETs is discussed in chapter 2. Previous studies on self-heating effects in nanoscale devices assumed a fixed boundary conditions at device level structure and solved the electronic and heat transport through an electro thermal solver. To study the heat removal from the device, package level structure has to be considered and relevant physics should be applied at micrometer length scales. Also heat removal from a device occurs at length scales that are orders of magnitude higher than the length scales important for the electronic transport (Phonon mean free path at 300K is about 300nm in bulk materials). Hence a multi scale simulator is necessary to properly understand the heat removal problem. In chapter 2, a multi scale simulator is developed and applied to the study of SHE in 22nm MOSFETS. Experimental data for the SHE of the structure is compared with the simulated model results. The developed model is in good agreement
with the experimental data at low applied biases but differs at higher biases. To explain the experimental behavior, the present model is being improved by improving the thermal solver with a Phonon Monte Carlo (PMC) solver. In chapter 3 a PMC solver is developed so as to couple with the electrical solver and better explain the experimental data.

The organization of the thesis is as following:

- Chapter 1 introduces the problem statement and explains the need for the study.

- In Chapter 2, a multi-scale simulator, as part of this research, is presented and applied to the case study of IMEC experimental setup on Self Heating Effects (SHE). The need to model the thermal transport with phonon Monte Carlo Simulator is elaborated in more details.

- Chapter 3 contains details about the development of phonon Monte Carlo simulator and its application for calculating the bulk thermal conductivity of silicon at different temperatures.

- Conclusions and future directions of research are presented in Chapter 4.
Chapter 2

ELECTRO-THERMAL MODELING

It is well-known that whenever a temperature gradient exists within a medium, thermal energy flows from a region of higher temperature to the one with lower temperature. This phenomenon is known as heat conduction and is described by the Fourier’s Law [7]

\[ \mathbf{q} = -\kappa \nabla T \]  

(2.1)

where \( \mathbf{q} \) is the heat flux vector, \( T \) is the local temperature, and \( \kappa \) is the thermal conductivity. If it is assumed that the local thermal energy can be described by the temperature, one can write a continuity equation for energy that involves the change of the local energy in time with the divergence of the heat flux given by Eq. (2.1)

\[ \nabla^2 T - \frac{1}{\alpha} \frac{dT}{dt} = -\frac{1}{\kappa} q_{\text{gen}} \]  

(2.2)

where \( q_{\text{gen}} \) is the heat generated. The thermal diffusivity \( (\alpha) \) is related to thermal conductivity \( (\kappa) \), the specific heat \( (c) \) and the density \( (\rho) \) by

\[ \alpha = \frac{\kappa}{\rho c} \]  

(2.3)

For steady state problems, the heat conduction equation simplifies to

\[ \kappa \nabla^2 T + q_{\text{gen}} = 0 \]  

(2.4)

In conventional electro-thermal simulations, it is common practice to associate the generated power density that appears in the above equation with Joule heating due to the presence of an electrical current and the resistivity of the material, i.e.

\[ q_{\text{gen}} = \mathbf{J} \cdot \mathbf{E} \]  

(2.5)
where \( \mathbf{J} \) is the local current density and \( \mathbf{E} \) is the local electric field, hence representing Joule heating as a local quantity. Generalizing to position dependent thermal conductivity, the heat conduction equation (2.4) can be expressed as

\[
\nabla \cdot (\kappa \nabla T) + \mathbf{J} \cdot \mathbf{E} = 0 \quad (2.6)
\]

In commercial device simulators, heat conduction equation is coupled to the Joule heating term with either the drift-diffusion or energy balance equations of the carriers. This then leads to the so-called non-isothermal drift-diffusion or energy balance models [8, 9, 10]. The coupling between the electron/hole transport in devices and the corresponding heat flow is achieved via temperature dependent mobilities and diffusion coefficients in the corresponding expression for current in Eq. (2.6). At one hand, the lattice temperature enters the expression for the local mobility value which, in turn, affects the electrostatics and current density in the device. On the other hand lattice temperature affects the local Joule heating term which, in turn, affects the lattice temperature profile. The electrical conduction and the heat flow equations are then self-consistently solved for the temperature and the electrostatic potential. A natural question then is: Is this self-consistent-solution model for electrical and thermal conduction within nanoscale devices valid when ballistic or non-stationary transport dominates and the mobility is no longer expressed by the classical picture? [11]

Many research groups have demonstrated that in nanoscale thermal transport, the use of simple Fourier law for heat conduction is inapplicable, rather the phonon Boltzmann Transport Equation must be solved directly to calculate accurately, for example, the thermal conductivity within thin films where boundary scattering plays significant role in the thermal conductivity degradation. This is needed in order to explain the already existing experimental data [12]. The length scale at which the Fourier heat law needs to be replaced with direct solution of the phonon Boltzmann
transport equation, in order to explain heat transport through nano-scale medium, is shown schematically in Fig. 2.1

![Figure 2.1: Length-scales and Relevant Thermal Transport Models](image)

The direct solution of the phonon Boltzmann transport equation is a very difficult task for a few reasons. First, it is difficult to express the anharmonic phonon decay processes mathematically. Second, one has to solve phonon Boltzmann equations for each individual mode of the acoustic and optical branches. A few attempts for solving the problem using the relaxation time approximation have been made by Narumanchi and co-workers[13]. If electrons and holes are included into the picture
with their corresponding Boltzmann transport equations, the solution of coupled set of equations, comprising the electron-hole-phonon system, becomes a formidable task even for modern day high performance computing systems.

Hence, some simplifications need to be made in order to solve this global problem. Since for device simulation purposes, we are only focused on calculating the I-V characteristics of a device accurately, the self-heating (which is a bye-product of the current flowing through the device) may be treated approximately, but still more accurately than the local heat conduction model. Starting from the principle of energy conservation, Majumder and co-workers derived separate energy balance equations for the optical phonon and the acoustic phonon bath[14, 15]. Under the application of electric fields greater than 10 kV/cm, electrons tend to lose energy primarily to optical phonons; optical phonons decay further to acoustic phonons. The energy conservation equations for optical and acoustic phonons are[16]

\[
\frac{\partial W_{LO}}{\partial t} = \left( \frac{\partial W_e}{\partial t} \right)_{coll} - \left( \frac{\partial W_{LO}}{\partial t} \right)_{coll} \tag{2.7}
\]

\[
\frac{\partial W_A}{\partial t} = \nabla (k_A \nabla T_A) \left( \frac{\partial W_e}{\partial t} \right)_{coll} + \left( \frac{\partial W_{LO}}{\partial t} \right)_{coll} \tag{2.8}
\]

where \( W_e, W_{LO} \) and \( W_A \) are electron, optical phonon and acoustic phonon energy densities respectively. Next, it is considered that

\[
dW_{LO} = C_{LO} dT_{LO} \tag{2.9}
\]

and

\[
dW_A = C_A dT_A \tag{2.10}
\]

where \( C_{LO} \) (specific heat capacity for optical phonons) can be estimated using the Einstein model while \( C_A \) (specific heat capacity for acoustic phonons) from the Debye
model. Next, the collision terms are expressed using the relaxation time approximation (RTA)

\[
\left( \frac{\partial W_e}{\partial t} \right)_{\text{coll}} = n \frac{3k_B T_e + \frac{1}{2} m^* v_d^2 - 3k_B T_{ph}}{\tau_{e-ph}},
\]

(2.11)

\[
\left( \frac{\partial W_{LO}}{\partial t} \right)_{\text{coll}} = C_{LO} \frac{T_{LO} - T_A}{\tau_{LO-A}},
\]

(2.12)

where \( T_e \) is the electron temperature, \( v_d \) is the electron drift velocity and \( T_{ph} \) can be optical or acoustic phonon temperature, depending on whichever kind of phonons the electrons interact with. Combining (2.7-2.12), one arrives at

\[
C_{LO} \frac{\partial T_{LO}}{\partial t} = \frac{3nk_B}{2} \left( \frac{T_e - T_{LO}}{\tau_{e-LO}} \right) + \frac{nm^* v_d^2}{2 \tau_{e-LO}} - C_{LO} \left( \frac{T_{LO} - T_A}{\tau_{LO-A}} \right),
\]

(2.13)

\[
C_A \frac{\partial T_A}{\partial t} = \nabla \cdot (\kappa_A \nabla T_A) + C_{LO} \left( \frac{T_{LO} - T_A}{\tau_{LO-A}} \right) + \frac{3nk_B}{2} \left( \frac{T_e - T_L}{\tau_{e-L}} \right).
\]

(2.14)

The first two terms on the right-hand side (RHS) of Eq. (2.13) represent the energy gained from the electrons, where \( n \) is the electron density, \( T_e \) is the electron temperature, \( v_d \) is the drift velocity and \( T_{LO} \) is the optical phonon temperature, while the last term is the energy lost to the acoustic phonons. The same term also appears as a gain term on the RHS of Eq. (2.14). While the first term on the RHS of Eq. (2.14) describes heat diffusion, the last term must be excluded if the electron-acoustic phonon interaction is considered to be elastic in nature. In this term, the lattice temperature, \( T_L \), is estimated as equivalent to the acoustic phonon temperature, \( T_A \).

For the case where the electric fields are less than 10 kV/cm, electrons lose energy directly to the acoustic phonons and in that case, the energy balance equations can be expressed as:

\[
C_A \frac{\partial T_A}{\partial t} = \nabla (\kappa_A \nabla T_A) + \left( \frac{\partial W_e}{\partial t} \right)_{\text{coll}}
\]

(2.15)
\[ C_A \frac{\partial T_A}{\partial t} = \nabla (\kappa_A \nabla T_A) - \frac{3nk_BT_A}{2\tau_{e-A}} + \frac{n\frac{3}{2}k_BT_e + \frac{1}{2}m^*v_d^2}{\tau_{e-A}} \] (2.16)

Under the assumption that at very low electric fields, the electron temperature and acoustic phonon temperatures equal the lattice temperature, the second and third terms in Eq (2.16) cancel. Using the low field conductivity and the mobility expressions, the heat source term in Eq (2.6) reduces to the last term of Eq (2.16) as below

\[ q_{\text{gen}} = J \cdot E = \sigma E^2 = \frac{\sigma v_d^2}{\mu^2} = \frac{n m^* v_d^2}{\tau}. \] (2.17)

It is assumed here that for low doping concentrations, the relaxation time, in Eq. (2.17), is the acoustic phonon relaxation time. The reason for this assumption is that acoustic phonon scattering process, being isotropic in nature, is very effective in randomizing the carrier momentum. The local Joule heating approximation Eq. (2.17) is, thus, valid for low fields, which is not the case in nanoscale devices.

While considering the electron-lattice coupling in (2.13-2.14), the energy transfer from energetic electrons to the optical phonons is very efficient. However, the optical phonons have very small group velocity and, therefore do not participate in the heat diffusion process effectively. Instead, they transfer their energy to acoustic phonons which can diffuse heat much more effectively. The energy transfer between phonons is a relatively slow process compared to the electron-optical phonon transport and therefore a thermal non-equilibrium condition may exist between optical and acoustic phonons. Fig. 2.2 shows the primary thermal energy transport path and the corresponding time constants[17]

In the current, state-of-the-art electro-thermal simulator, details of which can be found in section 2.1 below, steady-state versions of Eqs. (2.13) and (2.14) for the optical and acoustic phonon temperatures, respectively, are solved self-consistently
Figure 2.2: The Most Likely Path Between Energy Carrying Particles in a Semiconductor Device is Shown Together with the Corresponding Scattering Time Constants.

Courtesy of Ref. [17]

with a Monte Carlo simulation tool for the solution of the electron Boltzmann transport equation. This tool has been used to study self-heating in different technology nodes of nano-scale FD-SOI devices and dual gate device structures. As has already been explained, in smaller devices, non-stationary transport and velocity overshoot effect dominate the carrier transport, hence less degrading effect of self-heating on the on-current characteristics are observed.
2.1 ASU Model Description

In the research effort described herein, the EMC (Ensemble Monte Carlo) code for the carrier BTE solution has been modified as well (Fig. 2.3). As there are variable lattice temperatures in the hot-spot regions, the concept of temperature dependent scattering tables has been introduced. For each acoustic phonon temperature, one energy dependent scattering table is created. These scattering tables involve additional steps in the MC phase (see Fig. 2.4 right panel) since, in order to choose a scattering mechanism for a given electron energy randomly, it is necessary to know the corresponding lattice temperature dependent scattering table. To do that, first, the electron position on the grid needs to be known to retrieve the acoustic and optical phonon temperatures at that grid point. Then, the scattering table with coordinates \((T_L, T_{LO})\) is selected. Pre-calculation of the energy and temperature dependent scattering tables does not require much CPU time or memory resources. Also, the scattering table formation is done only once during the initialization of the simulation and is carried out for a broader range of temperatures. After the MC phase is complete, the electron temperature distribution and the average drift velocity and the carrier density at the node points are calculated. The exchange of variables between both solvers is shown on the left panel of Fig. 2.4

2.2 Multi-Scale Modeling of Circuits (CS and CD Configuration)

The International Technology Roadmap for Semiconductors (ITRS) suggests that as devices are scaled to smaller dimensions, the current density in the interconnects would increase \([18],[19]\). As has already been explained, due to the heat dissipated from the device, there is the potential for substantially increased temperature in critical regions of integrated circuits. Hence it is important to account for heating effects
Figure 2.3: Flowchart of the Electro-thermal Device Simulator - Coupling of the Monte Carlo Solver for the Electrons and the Energy Balance Equations for the Acoustic and Optical Phonons.

Courtesy of Ref. [16]
not only within the device itself, but also at the contacts and interconnects when considering reliability of a system. To do exactly that, a novel multi-scale simulation approach that combines circuit level simulations with device level simulations has been proposed. The approach compares simulation results with experimental measurements in an attempt to uncover the temperature profile due to self-heating effects.

The proposed method couples circuit level simulation performed using Silvaco Atlas [10] with an electro-thermal Monte Carlo device simulator [20]. The Giga3D Silvaco Atlas module simulates the thermal transport characteristics at the interconnect level. This module provides temperature boundary conditions for the device-level simulation. Then, the device level simulator solves for self-heating throughout the device. The coupled system is shown in Fig. 2.5. It is important to note that in the device
level thermal solver, the 2D/3D Poisson equation is solved self-consistently with a MC transport kernel coupled to a 2D/3D energy balance equations solvers for the acoustic (lattice) and optical phonon baths [21]. This is a new multi-scale approach which is very different from the commonly used Joule heating model used in commercial device simulators. Such simulations give rise to more pronounced hot-spots, because they accurately represent the optical to acoustic phonon bottleneck [22].
The device level temperature measurement technique used in this work is based on the temperature dependence of the sub-threshold slope of a planar MOSFET. The underlying idea is that variations in the sub-threshold slope in the sensor can be used to determine the temperature within the hot-spot of the device under test (DUT). The two devices are connected in either common source or common drain configuration. A sample of biasing conditions together with the schematics for both configurations is given in Fig. 2.6. Fig. 2.7 shows the mask image that indicates that both FETs that are located in a common active area and are separated by only one poly pitch.

![Figure 2.6: Two Possible Measurement Configurations are Common Source (Top) and Common Drain (Bottom). The Heater (DUT = Device Under Test) Operates in Saturation While the Sensor Operates in the Sub-threshold Region.](image)

The experimental procedure to estimate the hot-spot temperature was proposed by the IMEC group [23]. First, as schematically illustrated in Fig. 2.8, the increase
in temperature ($\Delta T$) induced by an nFET (i.e. the heater from Figs. 2.6 and 2.7) is extracted by making use of an nFET sensor that is located nearby this nFET or the device under test (DUT). This is done by using temperature dependent characteristics of the sensor. In this particular measurement setup the sensor is connected to a common source configuration with the heater (see Fig. 2.6). This configuration allows for the closest possible in silicon sensor since the two devices are separated only by one gate pitch. Also both these devices share the same active area which is surrounded by shallow trench isolation (see Fig 2.7). Subsequently, subthreshold slope (SS) in the sensor is extracted using a modified EKV model as illustrated in Fig. 2.8 [24].

The results from the experimental data are used as a reference for thermal simulations. The coupled solver uses the Monte Carlo method and the energy balance and Poissons equation to simulate the heating at the device level. The Joule heating,
defined as the product of the current density and the electric field, is extracted from these device-level simulations and used in the circuit level simulation. The Joule heating term is used as an input for the inter-connect level solver (Giga3D module within Silvaco Atlas framework). This Silvaco model provides the temperature boundary conditions at the device-level within the global electro-thermal device simulator. To integrate and interface these two separate modules, MATLAB is used (shown in Fig. 2.5).

The experimental transfer characteristic curves for drain voltages \( V_{DS} = 1, 1.5 \) and \( 2 \) V at the sensor are shown in Fig. 2.9. From the extracted subthreshold slopes, using the EKV method [24],[25] the corresponding average sensor temperatures for different bias conditions (\( V_{DS} \) and \( V_{GS} \)) are shown in Fig. 2.10. The goal of the multi-scale simulations is two-fold [26]: (1) Given the structure and the bias conditions in the heater-sensor configuration, the sensor temperature variation from Fig. 2.10 is reproduced (2). Once the sensor temperature match is achieved, extrapolation of the peak heater (DUT) temperature is performed. Hence the temperature of the hot-spot is uncovered in an indirect way.

To account for the heating at the source, gate and drain interconnects as shown in Fig. 2.5, first the complete circuit (device + interconnects) domain is solved using the Giga3D module of Silvaco Atlas. The temperature at the interconnects as well as the temperature in the device (along one cross-section) are shown in Fig. 2.11. At the boundaries of the rectangular cross-section from bottom panel in Fig. 2.11, lattice temperature is registered and used in the thermal particle-based device simulator which then provides: (1) the actual temperature of the hot-spot, and (2) the Joule heating terms that are used back in the Giga3D module for the next Gummel iteration (outer loop) of the model. It should be noted that solving the energy balance equations for acoustic and optical phonons self-consistently with the Boltzmann
transport equation for the electrons (that is solved using the MC method) is, by itself, a multi-scale problem [16]. Hence, in the implemented scheme we have three levels of abstraction. The convergence of the global Gummel loop is shown in Fig. 2.12.

The global loop converges within 5-10 Gummel cycles. In Figs. 2.13 and 2.14, the lattice (acoustic phonon) temperature and the optical phonon temperatures for the heater-sensor combination in the common-drain configuration (Fig. 2.6 (bottom panel)) are shown. Depending upon the applied bias, the lattice temperature profile obtained from Silvaco Atlas leads to an underestimation of the hotspot temperature by about 10-20K. Fig. 2.14 shows the bottleneck in the energy transport due to the low group velocity of the optical phonons. One can see a more localized hot-spot as compared to the acoustic (lattice) temperature case [27].

It is evident from the I-V curves shown in the Fig. 2.10 that the degradation of current is more at higher applied biases. The developed model predicts lower degradation. The model in the electro-thermal solver assumes heat transfer follow energy balance model and this may not be quite accurate for the present study. Thus the thermal solver has to be improved by directly solving the Phonon Boltzmann Transport Equation through the Monte Carlo technique. Before replacing the thermal solver, the Phonon Monte Carlo (PMC) solver should be developed, tested and validated. The testing and validation of the PMC solver is presented in Chapter 3.
Figure 2.8: Results for Two Instances of a Device. (Top Panel) the Subthreshold Swing (SS) Varies Linearly with the Externally Applied Chuck Temperature. (Middle Panel) When Drawing a Large Current Through the Heater, the SS of the Sensor Varies Linearly. (Bottom Panel) Using the Initial SS as a Reference, the Extracted $\Delta t$ in the Sensor Gives Consistent Results for Both Instances.
Figure 2.9: Measured Transfer Characteristics of the Sensor. Parameter is the Drain Voltage $V_{ds} = 1, 1.5$ and $2$ V.
Figure 2.10: Extrapolated and Simulated Average Sensor Temperature for Different Combinations of Drain and Gate Voltage
Figure 2.11: Giga3D Modeling of the Device + Interconnects (Top Panel). Extracted Lattice Temperature Boundary Conditions from Giga3D Simulations (Bottom Panel). Bias Conditions for the Common Drain Configuration Are: \( V_{s(DUT)} = 0, V_{d(Common)} = 1.5 \text{ V}, V_{g(DUT)} = 1.6 \text{ V}, V_{g(Sensor)} = 1.75 \text{ V} \) and \( V_{s(Sensor)} = 1.45 \text{ V} \).
Figure 2.12: Convergence of the Global Gummel Cycle (Loop)
Figure 2.13: Lattice Temperatures in the Heater (DUT) Sensor Configuration.
Figure 2.14: Optical Phonon Temperatures in the Heater (DUT) Sensor Configuration.
Phonon, in condensed-matter physics, is a unit of vibrational energy that arises from oscillating atoms within a crystal. Any solid crystal consists of atoms bound into a specific repeating three-dimensional spatial pattern called a lattice. Because the atoms behave as if they are connected by a tiny springs, their own thermal energy or outside forces make the lattice vibrate. This generates mechanical waves that carry heat and sound through the material. A packet of these waves can travel throughout the crystal with a definite energy and momentum, so in quantum mechanical terms the waves can be treated as a particle, called a phonon. A phonon is a definite discrete unit or quantum of vibrational mechanical energy, just as a photon is a quantum of electromagnetic or light energy. Phonons and electrons are the two main types of elementary particles or excitations in solids. Whereas electrons are responsible for the electrical properties of materials, phonons determine the speed of sound within a material and how much heat it takes to change its temperature.

The transport of phonons can be studied through the solutions of the Boltzmann Transport Equation (BTE) for phonons\[3\], that is of the form

$$\frac{\partial f}{\partial t} + v_g \cdot \nabla f = \left[ \frac{\partial f}{\partial t} \right]_{\text{scattering}}$$

(3.1)

where \(f\) is the distribution function of an ensemble of phonons, and \(v_g\) is the group velocity. The left hand side (lhs) of Eq. (3.1) represents the change of the distribution function due to motion whereas the right hand side (rhs) represents the change in the distribution function due to scattering. Motion causes the distribution function to deviate from equilibrium while scattering tends to restore equilibrium. Although the
motion of phonons is due to population gradient, it is popular to call this motion as drifting of phonons instead of diffusion of phonons[28]. The motion of phonons is referred to phonon drift in the present work.

An elegant way of solving the BTE is through the relaxation time approximation(RTA) where the scattering term on the rhs of Eq. (3.1) is approximated as

\[
\left[ \frac{\partial f}{\partial t} \right]_{\text{scattering}} = \frac{f - f_{eq}}{\tau}.
\]  

(3.2)

Here \( f_{eq} \) is equilibrium distribution under no forces and no gradients, \( \tau \) is the total relaxation time. The RTA implies that the system restores to equilibrium in an exponential form with a time constant equal to the total relaxation time. The total relaxation time depends on the scattering rates of different scattering mechanisms involved in the transport process. For heat conduction in crystals the scattering mechanisms are impurity scattering(or mass difference scattering), phonon boundary scattering and phonon-phonon scattering. The total scattering rate is then calculated through Matheissen’s rule as

\[
\tau^{-1} = \tau_{IM}^{-1} + \tau_{B}^{-1} + \tau_{Ph-Ph}^{-1}
\]  

(3.3)

where \( \tau_{IM}^{-1} \) is impurity scattering rate, \( \tau_{B}^{-1} \) is boundary scattering rate and \( \tau_{Ph-Ph}^{-1} \) is the phonon-phonon scattering rate. The RTA is only good when the deviation from the equilibrium is not very large. Also note that RTA is valid only when \( \tau \) is independent of the distribution function and the applied gradient.

Based on the momentum conservation of the phonons the phonon scattering mechanisms are classified into Normal(N) Process and Umklapp(U) Process. If the momentum is conserved (see Eq. (3.4)) in the scattering then the process is called N process. If the momentum is not conserved (Eq. (3.5)) then the process is called U process. In U processes the net momentum change is unit reciprocal lattice vector(\( \vec{G} \)).
The total energy is conserved in both processes.

\[ \vec{k}_1 + \vec{k}_2 = \vec{k}_3 \]  \hspace{1cm} (N Process) \hspace{1cm} (3.4)

\[ \vec{k}_1 + \vec{k}_2 = \vec{k}_3 + \vec{G} \]  \hspace{1cm} (U Process) \hspace{1cm} (3.5)

It is well known that the N processes try to shift the phonon distribution function towards high momentum in k-space while the U processes towards low momentum. When equilibrium is established between the two processes, it results in Bose-Einstein equilibrium distribution function for phonons. As temperature increases, the number of phonons undergoing N process and U process increases and new equilibrium is established. When a temperature gradient is present, then N processes (which favors for higher momentum) in higher temperature regions causes phonons to diffuse to lower temperature regions while U process (which favors for lower momentum) resists this diffusion which leads to finite thermal conductivity in the materials. U process is a resistive process for thermal conductivity. The impurity and boundary scattering are also resistive processes for thermal conductivity. For calculating the thermal conductivity only phonon-phonon scattering is considered in the present work.

3.1 Phonon-Phonon Scattering

Phonon-Phonon scattering is the dominant process involved in the heat conduction of materials. The scattering occurs because of anharmonic lattices forces between atoms in the crystal. Lattice forces between atoms are complicated functions of separation distance between atoms and can be expanded using Taylor series. When lattice forces are approximated as quadratic function of separation distance, the quantum mechanics theory leads to harmonic oscillator wave function states for atoms. Thus, when a lattice wave propagates, it carries energy only in discrete quanta of the energy states for atoms. This leads to the concept of phonons. Within the quadratic
approximation the phonons do not interact with each other[29]. When the Taylor series expansion include higher order terms the anharmonicity arises. Including cubic terms and applying first order perturbation theory results in three phonon interactions. With quartic terms four phonons interactions are possible. Developing expressions for scattering rates starting from the perturbing Hamiltonian is difficult. The frequency and the temperature dependence of the three phonon scattering rates are a strong function of the actual phonon branch and of the dispersion in the phonon spectrum. The approximated expressions may only be valid for certain types of phonons or for a limited temperature range[30]. Furthermore, the scattering processes are not necessarily independent and thus simple addition of scattering probabilities may not be justifiable. This has led to an experimental determination of analytical expressions for three phonon scattering rates. Such expressions for the relaxation times of scattering for Longitudinal Acoustic (LA) and Transverse Acoustic (TA) phonons are derived by Holland[30] and are of the form:

\[
\begin{align*}
\tau_{N,LA}^{-1} &= B_{LN} \omega^2 T^3 \\
\tau_{U,LA}^{-1} &= B_{LU} \omega^2 T^3 \\
\tau_{N,TA}^{-1} &= B_{TN} \omega T^4 \\
\tau_{U,TA}^{-1} &= \begin{cases} 
0 & \omega < \omega_{1/2} \\
\frac{B_{TU} \omega^3}{\sinh \left( \frac{\omega}{\tau_{BU}} \right)} & \omega > \omega_{1/2} 
\end{cases}
\end{align*}
\]

where \( \omega_{1/2} \) is the TA phonon frequency corresponding to \( K/K_{max} = 0.5 \) and \( B_{LN}, B_{LU}, B_{TN} \) and \( B_{TU} \) are constants for a given material. The values for Si are listed in Table 3.1. The scattering rates for Longitudinal Optical (LO) and Transverse Optical (TO) phonons are ignored mainly because of their low group velocities. Recent studies [3, 31] suggested that optical phonons must be considered in the steady state thermal conductivity predictions. Using the method described by Han and Klemens [32],
Narumanchi et al. [13] derived the scattering rates of U processes both for acoustic modes as well as optical modes. The scattering rates of U processes involving only acoustic phonons of type Eq. (3.10) is given by Eq. (3.11). In Eq. (3.10) BZB refers to Brillouin Zone Boundary.

\[ \text{LA} + \text{TA}(BZB) \leftrightarrow \text{LA}; \text{ TA} + \text{TA}(BZB) \leftrightarrow \text{LA}; \text{ TA} + \text{LA}(BZB) \leftrightarrow \text{LA} \] (3.10)

\[ \tau_{ij}^{-1} \approx \frac{\chi \gamma^2 \hbar}{3 \pi \rho v_{ph}^2 v_g} \omega_i \omega_{tr} \omega_j \tau_c \left[ \frac{1}{e^{\hbar \omega_{tr}/k_B T} - 1} - \frac{1}{e^{\hbar \omega_j/k_B T} - 1} \right] \] (3.11)

where the indexes refers to phonons interactions of type given by Eq. (3.12). Incoming phonon \( (Ph_i) \) interacts with translated phonon \( (Ph_{tr}) \) resulting in outgoing phonon \( (Ph_j) \)

\[ Ph_i + Ph_{tr} \leftrightarrow Ph_j \] (3.12)

In Eq. (3.11), \( \chi \) is the degeneracy of translated mode phonon, \( v_g(= |\partial \omega_j/\partial q_j|) \) is the group velocity of outgoing phonon, \( v_{ph}(= \omega_i/q_i) \) is the phase velocity of the incoming phonon, \( \gamma \) is the Gruneisen constant with value of 0.59[3] for silicon, \( \rho \) is the density
of the material (here Si) and \( r_c \) is the effective radius

\[
r_c = \frac{2\pi / a - k_i}{2\sqrt{2}}.
\]  

(3.13)

In Eq. (3.13), \( a \) is the lattice constant of Si, \( k_i \) is the wavevector of incoming phonon.

For the interactions of type given by Eq. (3.14) involving optical phonons (indexing same as in Eq. (3.12)), the scattering rate is given by Eq. (3.15)

\[
LA/TA + LA/TA \leftrightarrow LO/TO(BZB)
\]  

(3.14)

\[
\tau_{ij}^{-1} \approx \frac{\chi^2 \hbar}{3\pi \rho \nu^2 \nu g^3 \omega_{ji} \omega_{ji} \omega_{tr}^3} \left[ \frac{1}{e^{\hbar \omega_{ji} / k_B T} - 1} - \frac{1}{e^{\hbar \omega_{ji} / k_B T} - 1} \right]
\]  

(3.15)

where all the symbols have the same meaning as in Eq. (3.11) except \( v_g \). In Eq. (3.15) \( v_g \) is the group velocity of the translated mode phonon i.e. \( v_g = \partial \omega_{tr} / \partial q_{tr} \).

The phonon-phonon scattering processes that are believed to be important in thermal conductivity calculations[3] are listed in Table 3.2

Assuming that the scattering processes are independent, the total scattering rates of different three phonon processes of type given in Eq. (3.10) and Eq. (3.14) can be added using Matheissen rule and the scattering rate for U process is then given as

\[
\tau_{U,i}^{-1} = \sum_j \tau_{ij}^{-1}
\]  

(3.16)

Mittal and Mazumder[3] used hybrid approach to calculate the thermal conductivities of silicon thin films. They used Hollands expressions for N processes and Eq. (3.11), Eq. (3.15), Eq. (3.16) for U processes.

In a recent paper, Kazan et al. [33] used analytical expressions similar to those of Hollands except that the scattering rate constants are not calibrated from experiments.
<table>
<thead>
<tr>
<th>Longitudinal Acoustic Phonons</th>
<th>Transverse Acoustic Phonons</th>
</tr>
</thead>
<tbody>
<tr>
<td>LA + TA(BZB) ↔ LA</td>
<td>TA + TA(BZB) ↔ LA</td>
</tr>
<tr>
<td>LA + TA ↔ LO(BZB)</td>
<td>TA + LA(BZB) ↔ LA</td>
</tr>
<tr>
<td>LA + TA ↔ TO(BZB)</td>
<td>TA + LA ↔ LO(BZB)</td>
</tr>
<tr>
<td>LA + LA ↔ LO(BZB)</td>
<td>TA + LA ↔ TO(BZB)</td>
</tr>
<tr>
<td>LA + LA ↔ TO(BZB)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Longitudinal Optical Phonons</th>
<th>Transverse Optical Phonons</th>
</tr>
</thead>
<tbody>
<tr>
<td>LO ↔ LA + TA(BZB)</td>
<td>TO ↔ LA + TA(BZB)</td>
</tr>
<tr>
<td>LO ↔ LA + LA(BZB)</td>
<td>TO ↔ LA + LA(BZB)</td>
</tr>
<tr>
<td>LO ↔ TA + LA(BZB)</td>
<td>TO ↔ TA + LA(BZB)</td>
</tr>
</tbody>
</table>

Table 3.2: Important Three Phonon Interaction for U-process

but determined through material constants. The scattering rates are given by

\[
\tau_{N,LA}^{-1} = B_{LN} \omega^2 T^3
\]

\[
\tau_{U,LA}^{-1} = B_{LU} \omega^2 T e^{-\theta_{DL} / 3T}
\]

\[
\tau_{N,TA}^{-1} = B_{TN} \omega T^4
\]

\[
\tau_{U,TA}^{-1} = B_{TU} \omega T e^{-\theta_{DT} / 3T}
\]

with

\[
B_{LN} = \frac{k_B^2 \gamma_L^2}{\rho \hbar^2 v_L^5}
\]

\[
B_{LU} = \frac{\hbar \gamma_L^2}{M_L^2 \theta_{DL}}
\]

\[
B_{TN} = \frac{k_B^4 \gamma_T^2}{\rho \hbar^2 v_T^5}
\]

\[
B_{TU} = \frac{\hbar \gamma_T^2}{M_T^2 \theta_{DT}}
\]
<table>
<thead>
<tr>
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<th>Units</th>
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</thead>
<tbody>
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<td>$v_T$</td>
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<td>m/s</td>
</tr>
<tr>
<td>$v_L$</td>
<td>8430</td>
<td>m/s</td>
</tr>
<tr>
<td>$\theta_{DT}$</td>
<td>240</td>
<td>K</td>
</tr>
<tr>
<td>$\theta_{DL}$</td>
<td>586</td>
<td>K</td>
</tr>
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</table>

Table 3.3: Material Parameters for Calculating Scattering Constants
(Data From [33])

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma_L$</td>
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<td>no units</td>
</tr>
<tr>
<td>$\gamma_T$</td>
<td>0.6</td>
<td>no units</td>
</tr>
<tr>
<td>$B_{TU}$</td>
<td>$1.0 \times 10^{-19}$</td>
<td>$s^{-1}K^{-3}$</td>
</tr>
<tr>
<td>$B_{LU}$</td>
<td>$5.5 \times 10^{-20}$</td>
<td>$s^{-1}K^{-3}$</td>
</tr>
<tr>
<td>$B_{TN}$</td>
<td>$7.1 \times 10^{-13}$</td>
<td>$s^{-1}K^{-5}$</td>
</tr>
<tr>
<td>$B_{LN}$</td>
<td>$2.4 \times 10^{-24}$</td>
<td>$s^{-1}K^{-5}$</td>
</tr>
</tbody>
</table>

Table 3.4: Material Parameters for Calculating Scattering Constants
(Data From [34])

where $v_L, v_T$ are group velocity of LA,TA phonons at Brilluoin Zone centre, $\theta_{DL}, \theta_{DT}$ are the Debye temperature for LA,TA phonons, $\gamma_L, \gamma_T$ are Gruneisen constants for LA,TA phonons. The values taken from [33] are listed in Table 3.3 The values for Gruneisen constants and scattering rate constants taken from [34] are summarized in Table. 3.4

In the present work thermal conductivity calculations are performed in 3 ways. Within the first method, Holland expressions are used and thermal conductivities of

33
silicon are calculated without including optical phonons. In second approach Mittal and Mazumder hybrid method is used to calculate thermal conductivities of silicon with and without the inclusion of optical phonons. Third method utilizes Kazan et al. expressions to calculate thermal conductivities of silicon without optical phonons. All the results are compared with experimentally measured thermal conductivities of silicon by Glassbrenner and Slack [35].

3.2 Monte Carlo Simulation Procedure

Here, the phonon BTE is solved in the relaxation-time approximation using the Monte Carlo method. Direct method for solving the phonon BTE exists, but treating different scattering mechanisms independently is very difficult. Also incorporation of new scattering mechanism is complicated. The formalism for direct solution method of the phonon BTE can be found in [33].

The main advantages of using Monte Carlo technique[28] are

- simple treatment of transient problem,

- ability to consider complex geometry, and the

- possibility to follow each scattering process independently.

Monte Carlo method provides good insights about the physical nature of the transport problem. New scattering mechanisms can be easily incorporated into the simulation code without much difficulties.

The main steps involved in Monte Carlo solution method for phonon BTE are:

- Input geometry and boundary conditions.

- Input material constants and dispersion relation.

- Calculate scattering, polarization, distribution and weighted distribution tables.
- Initialize phonons in the simulation domains (cells) with distribution tables.

- Free flight the phonons.

- Calculate new temperature ($\bar{T}$).

- Scatter phonons with scattering rates at $\bar{T}$.

- Using weighted distribution tables add or delete phonons (Reinitialization).

- Calculate phonon flux flow in all cells.

- Thermalize the end cells with boundary temperature conditions.

### 3.2.1 Geometry and Boundary Conditions

Before the simulation begins, the geometry for the simulation domain has to be decided. Once the geometry is decided the simulation domain is partitioned into cells. The cells touching the boundaries are termed as thermal boundary cells. The boundary conditions set the temperature of the boundary cells. Other cells, which are not boundary cells have adiabatic boundary conditions and hence are termed as adiabatic boundary cells. The phonons which reach the thermal boundary cells are thermalized to boundary temperature. The phonons in the adiabatic boundary cells reaching the side boundaries as specularly reflected. If boundary scattering is incorporated this has to be changed to partially specular and partially diffusive reflection. In the present work boundary scattering is not being modeled.

The geometry chosen in the current study is a simple cubic cell stack as shown in Fig. 3.1. The current Monte Carlo method solves the phonon transport in 1 dimension (along Z-direction) in silicon slab with dimensions $L_x = 50\text{nm}$, $L_y = 50\text{nm}$, $L_z = 400\text{nm}$ and $N = 20$. The boundary conditions are given by $T_h = T + 10K$
and $T_c = T - 10K$ where $T$ is the temperature at which the thermal conductivity calculation is done.

![Geometry of the Structure Chosen for Simulation in the Present Study](Figure 3.1)

(Courtesy of Ref. [28])

3.2.2 Material Constants and Dispersion Relations

All the material constants, including the scattering rate constants, are inputted to the simulator. The material chosen in this work is silicon.

The dispersion of the material should be known for each phonon branch. The full band dispersion of silicon is not incorporated in the present work. Assuming isotropic Brillouin Zone (BZ) approximation, the experimental phonon dispersion for silicon is fitted with quadratic curve [36] fit as

$$\omega_k = \omega_0 + v_s k + ck^2$$  \hspace{1cm} (3.25)

For acoustic modes, the constants $v_s$ and $c$ are chosen so as to capture the slope of the dispersion curve near the center of the BZ and maximum at the edge of BZ. For longitudinal optical phonons, they ensure LO frequency at BZB equals the maximum frequency of LA. For both TA and TO phonons, the curves are fitted such that the
slopes at the BZ edge are zero [17]. The curve fit parameters for silicon are shown in Table 3.5. The dispersion of silicon with the curve fitting is as shown in Fig. 3.2 From the dispersion relation group velocities for the phonons are calculated using

\[ v_g = \frac{\partial \omega}{\partial k} = v_s + 2ck \quad (3.26) \]

These constants are inputted into the Monte Carlo code. In the present study, since isotropic BZ is assumed, the direction of the group velocity will be same as the direction of the wave vector \( k \).

### 3.2.3 Scattering, Polarization and Distribution Tables

In the previous studies on Phonon Monte Carlo simulations [37, 38] the scattering rates, probability of scattering, probability for polarization and probability for phonon modes are all calculated on the fly during the simulation. The disadvantage of this method is that adding new scattering mechanism and including optical modes becomes difficult. A better way of simulating is to calculate tables for scattering rates, scattering probabilities, polarization probabilities and distribution probabilities. All the tables are functions of phonon frequencies and lattice temperatures. Hence the

<table>
<thead>
<tr>
<th>Phonon Type</th>
<th>( \omega_0 ) ((10^{13} \text{ rad/s}))</th>
<th>( v_s ) ((10^{3} \text{ m/s}))</th>
<th>( c ) ((10^{-7} \text{ m}^2/\text{s}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>LA</td>
<td>0.00</td>
<td>9.01</td>
<td>-2.01</td>
</tr>
<tr>
<td>TA</td>
<td>0.00</td>
<td>5.23</td>
<td>-2.26</td>
</tr>
<tr>
<td>LO</td>
<td>9.88</td>
<td>0.00</td>
<td>-1.60</td>
</tr>
<tr>
<td>TO</td>
<td>10.20</td>
<td>-2.57</td>
<td>1.12</td>
</tr>
</tbody>
</table>

Table 3.5: Curve-fit Parameters for Silicon Dispersion Data

(Data from Ref. [36])
frequency of phonons from 0 to $\omega_{\text{max}}$ is divided into 1000 bins and lattice temperature from $T_h + 10K$ to $T_c - 10K$ into 1000 bins. Let $i$ denote the index for phonon frequency bin and $j$ denote the index for lattice temperature bin. First the spectral distribution of phonons at each temperature bins for each phonon mode is calculated and stored. The number of phonons of a given type $t$ (acoustic or optical) with a given polarization $p$ (longitudinal or transvers) in a volume of $V$ within the spectral bin $\omega$ to $\omega + \Delta\omega$ at a given temperature $T$ with isotropic approximation is given by

$$N_{t,p} = \left[ \frac{1}{e^{\left(\frac{\hbar c_{t,p}}{k T_j}\right)} - 1} \right] \frac{k^2_{t,p}}{2\pi^2 v_{g,t,p}} \chi_{t,p} \Delta\omega.$$ (3.27)
Here $k_{t,p}$ wavevector of the phonon, $\chi_{t,p}$ degeneracy of the phonon (because of isotropic assumption), $v_{g,t,p}$ group velocity of phonon. Hence

$$N_{\text{type}}(i,j) = \left[ \frac{1}{e \left( \frac{\hbar v_{g,t,p}}{k_B T} \right)} - 1 \right] \frac{k_{t,p}^2}{2\pi^2 v_{g,t,p}^2} \chi_{\text{type}} \Delta \omega$$

for type=LA,TA,LO,TO (3.28)

The spectral distribution of phonon is needed to build the cumulative number distribution tables. Next, cumulative number distribution table is calculated as

$$F(i,j) = \sum_{ii=1}^{N} \frac{N_{\text{tot}}(i,i,j)}{N_{\text{tot}}(i,j)}$$

where $N_b$ is the total number of frequency bins (1000) and $nT_{\text{tot}}(i,j)$ is given as

$$N_{\text{tot}}(i,j) = N_{\text{LA}}(i,j) + N_{\text{TA}}(i,j) + N_{\text{LO}}(i,j) + N_{\text{TO}}(i,j)$$

(3.30)

This cumulative number distribution table is used during the initialization of phonons to decide the frequency for phonon so that they follow Bose-Einstein statistics. The use of this table is discussed in the initialization section.

An energy table is also calculated as

$$E(j) = \sum_{i=1}^{N_b} N_{\text{tot}}(i,j) \hbar \omega_i \ast V_{\text{cell}}$$

(3.31)

where $V_{\text{cell}}$ is the volume of the cell.

The polarization probability table is calculated as

$$P(i,j,1) = \frac{N_{\text{LA}}(i,j)}{N_{\text{tot}}(i,j)}$$

(3.32)

$$P(i,j,2) = \frac{N_{\text{LA}}(i,j) + N_{\text{TA}}(i,j)}{N_{\text{tot}}(i,j)}$$

(3.33)

$$P(i,j,3) = \frac{N_{\text{LA}}(i,j) + N_{\text{TA}}(i,j) + N_{\text{LO}}(i,j)}{N_{\text{tot}}(i,j)}$$

(3.34)
The polarization table is useful during initialization to determine type and polarization of the initialized phonon. The procedure to determine the polarization of the phonon is discussed in initialization.

Using the scattering rates given in Eq. (3.6)-(3.20) the scattering table is calculated as

\[ S_{\text{type}} = \frac{\tau_{N,\text{type}}^{-1}(i, j)}{\tau_{N,\text{type}}^{-1}(i, j) + \tau_{U,\text{type}}^{-1}(i, j)} \text{ for type}=\text{LA,TA,LO,TO} \] (3.35)

The scattering table is used during scattering of phonons to determine the type of scattering process a phonon would undergo in a scattering event. This is discussed in the scattering section.

Also, the probability table for being scattered within \( \Delta t \) of simulation time is calculated as

\[ p_{\text{Scat type}}(i, j) = 1 - \exp \left( -\frac{\Delta t}{\tau_{N,\text{type}}^{-1}(i, j) + \tau_{U,\text{type}}^{-1}(i, j)} \right) \text{ for type}=\text{LA,TA,LO,TO}. \] (3.36)

These tables are required during the scattering of phonons to decide whether a given type of phonon would undergo a scattering event. They are also used to calculate the weighted distribution and polarization tables.

The weighted cumulative distribution function is calculated as

\[ F_w(i, j) = \sum_{i=1}^{i} \frac{N_{\text{tot,w}}(i, j)}{N_r} \] (3.37)

where \( N_{\text{tot,w}}(i, j) \) is given by

\[ N_{\text{tot,w}}(i, j) = \sum_{\text{type}=\text{LA,TA,LO,TO}} N_{\text{type}}(i, j) p_{\text{Scat type}}(i, j). \] (3.38)

The weighted probability distribution function is calculated as

\[ P_w(i, j, 1) = \frac{N_{\text{LA}}(i, j) p_{\text{Scat LA}}(i, j)}{N_{\text{tot,w}}(i, j)}, \] (3.39)
\[ P_w(i, j, 2) = \frac{N_{LA}(i, j) pScat_{LA}(i, j) + N_{TA}(i, j) pScat_{TA}(i, j)}{N_{tot,w}(i, j)}, \]  
\[ P_w(i, j, 3) = \frac{N_{LA}(i, j) pScat_{LA}(i, j) + N_{TA}(i, j) pScat_{TA}(i, j) + N_{LO}(i, j) pScat_{LO}(i, j)}{N_{tot,w}(i, j)}. \]  

These tables are used in re-initialization of phonons. The need for these tables is discussed in the scattering section and how they are used is discussed in re-initialization section.

### 3.2.4 Initialization

After building scattering, distribution, polarization and weighted distribution tables, the phonons in each cell have to be initialized with position vector, wave vector, frequency, group velocity and type of phonon. To do so, the total number of phonons in each cell should be known. The total number of phonons in a cell at T can be calculate as

\[ N_{\text{tot}} = \sum_{i=1}^{N_b} N_{\text{tot}}(i, j) \times V_{\text{cell}} \]  

where \( V_{\text{cell}} \) is the volume of cell, \( j \) is the index of the bin within which T lies i.e., T lies between bin \( j \) and bin \( j+1 \).

The total number of phonons in each cell is very large (for example the number of phonons in a cell of dimension 50nm x 50nm x 200nm slab of silicon at 300K is about 31 million). Hence a weighting factor is used to scale down this number[39].

After fixing the number of phonons, the following is done until the total energy within the cell matches with the calculated energy \( E(j) \) to initialize each phonon:

- Get a random number \( r \) between 0 and 1.

- Find the index \( i \) such that \( F(i, j) < r < F(i + 1, j) \) where \( j \) is fixed by the temperature of the cell.
- Set the frequency of phonon as

\[ \omega = \omega_i + (2r - 1) \frac{\Delta \omega}{2} \]

- Get another random number \( r \) between 0 and 1.

- Find the index \( ii \) such that \( P(i, j, ii) < r < P(i, j, ii + 1) \)

- Based the value of \( ii \) set the type of phonon

\[
\begin{align*}
    type &= LA & \text{if } ii = 0 \\
    type &= TA & \text{if } ii = 1 \\
    type &= LO & \text{if } ii = 2 \\
    type &= TO & \text{otherwise}
\end{align*}
\]

- Using the dispersion relation corresponding to the type of phonon, calculate the magnitude of \( q \) vector and set the group velocity \( v_g \) for the phonon at that \( q \)

- Get another random number \( r \) between 0 and 1.

- Fix \( \theta \) such that \( \cos(\theta) = 2r - 1 \).

- Get another random number \( r \) between 0 and 1.

- Fix \( \phi \) such that \( \phi = 2\pi r \).

- Set the \( q \) vector components as

\[
\begin{align*}
    q_x &= q \sin(\theta) \cos(\phi) \\
    q_y &= q \sin(\theta) \sin(\phi) \\
    q_z &= q \cos(\theta)
\end{align*}
\]

\( (3.43) \)
• Initialize the position such that the phonon will be within the boundary of the cell.

The above procedure ensures that the initialized phonons follow Bose-Einstein statistics and have zero net momentum.

3.2.5 Free-Flight of Phonons

After initialization, free-flight and scattering of phonons is done until the end of the simulation time. During the free-flight the phonons are allowed to move within the cell with a corresponding group velocity $v_g$. The phonon position is updated after a time of $\Delta t$ as

$$\vec{r}_{\text{new}} = \vec{r}_{\text{old}} + \vec{v}_g \cdot \Delta t$$  \hfill (3.44)

If the phonons cross the boundary in X or Y direction then they are reflected (adiabatic boundary) and the corresponding momentum direction sign is reversed. If the phonons cross the boundary in Z direction then it is marked so as to delete it in the present cell and update it into new cell. The marked phonons are also useful to calculate the flux flowing in and out of each cell. All the cells are updated at the end of free-flight of phonons with the drifted phonons.

3.2.6 New Temperature Calculation ($\tilde{T}$)

After the free-flight of phonons is completed, the total energy of the cell will change because of the drift. This means the phonon distribution is also changed. Assuming the new phonon distribution is near to Bose-Einstein equilibrium distribution a new temperature ($\tilde{T}$) is calculated such the total energy of the cell is same as the total energy of the equilibrium phonon distribution at $\tilde{T}$. The calculation is done by numerically inverting the Eq. (3.31). Since energy table gives the table energy for
a given temperature, a simple search will give the value for $\tilde{T}$. Once the value of $\tilde{T}$ is known it is used to find the scattering rates, probability of scattering of phonons during the scattering event. This is explained in the next section.

### 3.2.7 Scattering of Phonons

In this work, phonon-phonon scattering is treated as a three phonon phenomena. When a phonon gets scattered it either combines with second phonon and give third phonon or decays into two phonons. In either cases a scattering event transform a phonon to another phonon along with addition of new phonon or deletion of old phonon. Addition happens when it decays to two phonons and deletion happens when it combines to give third phonon. Also, the energy and net momentum are conserved. So every scattering event requires a selective addition or deletion of phonon from the simulation domain. A search for such selective phonons in the simulation domain is computationally very expensive. To avoid this, previous studies on phonon Monte Carlo methods[3, 28, 40] provided an approximate method of simulating the scattering event.

It is well known that a scattering events tend to restore equilibrium. Since scattering is done after every $\Delta t$ time which is chosen such that $\Delta t > 3\tau_{\text{max}}$, 95% of the system will be restored to equilibrium. This is because the relaxation time approximation shows the system will restore equilibrium in exponential decay fashion with time constant $\tau$ and hence within 3 time constants 95% will be restored. Thus, the system in near equilibrium at $t$ and $t + \Delta t$. Mazumder and Majumdar[40] suggested that instead of adding or deleting phonons one at a time during each scattering event, mark all the phonons that are going to scatter. After marking redistribute only the marked phonons such that they follow equilibrium statistics at $\tilde{T}$. Add or delete phonons until the total energy is conserved. The procedure is summarized as below.
1. For each phonon in the cell, find the type, frequency (i.e., bin index $i$) of phonon.

2. Get a random number $r$ between 0 and 1.

3. Mark the phonon if $r$ is greater than $p_{\text{Scatt}}(i, j)$ where $j$ refers to temperature bin index corresponding to $\bar{T}$.

4. For each marked phonon, get a random number between 0 and 1.

5. Find the index $ii$ such that $F(ii, j) < r < F(ii + 1, j)$ ($j$ is for $\bar{T}$).

6. Change the state of phonon from bin $i$ to $ii$ by resetting the momentum and group velocity. (Position remains the same)

7. Calculate the gain of energy as $\hbar(\omega_{ii} - \omega_i)$.

8. Calculate the net gain of energy by summing the gain of all marked phonons.

9. If the net gain is negative add the phonons just like initialization until the net gain is zero.

10. Else, delete phonons by drawing random number between 0 to $N_{\text{cell}}$ until the net gain is zero. ($N_{\text{cell}}$ is the number of phonons in the cell).

Later Lacroix et al. [28] changed the distribution function $F(i, j)$ to weighted or modulated distribution function $F_{w}(i, j)$ in order to have the rate of creation of phonons into a state equal to its rate of destruction. It can be understood by carefully analyzing the Eq. 3.2 which can be rewritten as [33]

$$\left[ \frac{\partial N}{\partial t} \right]_{\text{scattering}} = \frac{N - \bar{N}_{eq}}{\tau_{\text{tot}}} \tag{3.45}$$

$$\implies \Delta N(t) = \Delta N(0)e^{-\frac{t}{\tau_{\alpha}}} \tag{3.46}$$
\[ N_{t+\Delta t} - \bar{N}_{eq} = \left( N_t - \bar{N}_{eq} \right) e^{-\frac{\Delta t}{\tau_{tot}}} \]  

(3.47)

\[ N_{t+\Delta t} = \bar{N}_{eq} \left( 1 - e^{-\frac{\Delta t}{\tau_{tot}}} \right) + N_{Dri,ft} e^{-\frac{\Delta t}{\tau_{tot}}} \]  

(3.48)

Note that Eq. 3.47 is written for the scattering events between \( t \) and \( t + \Delta t \) and in Eq. 3.48 \( N_t \) is nothing but the spectral distribution obtained after the drifting of phonons at time \( t \) which is denoted as \( N_{Dri,ft} \). Mazumder and Majumdar[40] argument is choosing \( t > 3 \times \tau_{tot} \) would have \( e^{-\frac{\Delta t}{\tau_{tot}}} \rightarrow 0 \) and hence the distribution at \( t + \Delta t \) would be equilibrium distribution at \( \bar{T} \). Lacroix argument is approximate in a sense that only the drift term exponential to zero and exponential in equilibrium (which is nothing but probability of scattering) should not be ignored. Hence the equilibrium distribution is modulated/weighted with the probability of scattering.

In scattering routine only marking of phonons is done. The task of adding phonon and deleting phonon is completed by reinitialization routine.

### 3.2.8 Reinitialization

Once the phonon is marked to undergo scattering, the act of adding or deleting the phonon is completed by reinitialization routine performing the steps from 5 to 10 listed in the scattering section. The reinitialization is performed only for scattered phonons but not for all the phonons in the cell. The scattering for boundary cells is not calculated as they should be thermalized to the boundary conditions but drifting of phonons is done for boundary cell.

### 3.2.9 Phonon Flux Calculation

During the drifting of phonons, the phonons which cross the boundary are marked. If the phonons are moving out from cell\(_i\) to cell\(_{i+1}\) then the net flux crossing is added to cell\(_i\). If the phonons are moving out from cell\(_{i+1}\) to cell\(_i\), then the net flux crossing
is subtracted from cell $i$. The net flux calculation is done with the following expression.

$$\text{flux } (\Phi_i) = \left( \sum_{\text{cell}_{i-1} \rightarrow \text{cell}_i, \text{all phonons } j} \hbar \omega_j \frac{q_{j,i}}{|q_j|} - \sum_{\text{cell}_{i} \rightarrow \text{cell}_{i+1}, \text{all phonons } j} \hbar \omega_j \frac{q_{j,i+1}}{|q_j|} \right) / (\Delta t A) \quad (3.49)$$

where $A$ is the area of cross section ($= L_x \times L_y$)

The calculated cell flux and temperature are written to a file and the thermal conductivity is calculated from the expression

$$\kappa = -\left\langle \frac{\Phi_i}{\Delta T_i / \Delta z} \right\rangle \quad (3.50)$$

### 3.2.10 Thermalization of Boundary Cells

The boundary cells are thermalized to the boundary cell temperature. All the phonons in the boundary cell are initialized like normal initialization but at boundary cell temperature. This is repeated for every $\Delta t$ time step of the simulation.

### 3.3 Verification of Monte Carlo Code

The Monte Carlo steps are implemented in fortran language. The basic framework for the PMC is taken from Edwin Ramayya’s work[37] and has been modified to implement the scattering tables and optical phonons transport for heat conduction. First the input material properties for the silicon are verified by plotting the dispersion curves and group velocity curves. The dispersion curves for TA, LA, TO and LO phonons calculated from this work and Mittal’s work[3] are as shown in Fig. 3.3. The corresponding group velocities are compared in Fig. 3.4
Figure 3.3: Comparison of Dispersion Curves for Silicon
Data from Mittal’s Work [3]

Figure 3.4: Comparison of Group Velocities of Silicon
Data from Mittal’s Work[3]
Next the cumulative distribution function (CDF) curve is verified. Since these CDF curves only depend on dispersion curves and Bose-Einstein distribution, they are independent of scattering rates and the results from different works can be compared for verification. The CDF with optical phonons at different temperatures comparing with Mittal’s work [3] is as shown in Fig. 3.5. The CDF without optical phonons at different temperatures comparing with Mittal’s work [3] is as shown in Fig. 3.6.

![Comparison of CDF at different temperatures with optical phonons](image)

**Figure 3.5:** Comparison of Cumulative Distribution Function at Different Temperature with Optical Phonons

Data from Mittal’s Work [3]
Figure 3.6: Comparison of Cumulative Distribution Function at Different Temperature Without Optical Phonons

Data from Mittal’s Work [3]

Noting that there is a slight difference in the Mittal’s result and the current work, another comparison for the CDF without optical phonons is done with data from Lacroix[28]. Fig. 3.7 and Fig. 3.8 shows the CDF at 300K and 500K of the present work compared with data extracted from Lacroix[28].
Figure 3.7: Comparison of CDF at 300K Without Optical Phonons

Data from Lacroix’s Work [28]

Figure 3.8: Comparison of CDF at 500K without optical phonons

Data from Lacroix’s Work [28]
The next set of data verified is the scattering rates. As discussed earlier the scattering rates are calculated in 3 different ways. Using the Holland’s expression scattering times at 100K and 300K are plotted in Ref [3]. These scattering times are compared with the present work scattering time calculations and are shown in Fig. 3.9(300K) and Fig. 3.10(100K).

Figure 3.9: Scattering Times Comparison at 300K

Data from Mittal’s Work [3]
Figure 3.10: Scattering Times Comparison at 100K

Data from Mittal’s Work [3]
For Monte Carlo particle based simulations one observed behavior is the shift of drift velocity from zero along the direction of the flow of particles. Applying a gradient of 400K around 300K ($T_c=100K$ and $T_h=500K$) in the z-direction, the average velocity of the phonons are as shown in Fig. 3.11

![Graphs showing average drift velocities in X, Y, and Z-directions with applied gradient of 400K](image)

Figure 3.11: Average Drift Velocities of Phonons in X, Y and Z-direction When a Gradient of 400K Is Applied along Z-direction
3.4 Results

In this section, the results for the scattering tables, polarization tables and distribution tables are presented. The tables depend on temperature and frequency of the phonons. The plots of the table at 300K are presented in this section and the plots at 100K and 900K are presented in the appendix A.

The total scattering times calculated with three different approaches at 300K is as shown in Fig. 3.16. The cumulative and weighted cumulative distribution functions at 300K is as shown in Fig. 3.16 and Fig. 3.13 respectively. The results for polarization tables and modulated polarization tables are as shown in Fig. 3.14 and Fig. 3.15 respectively. From the scattering time plots it is clear that high frequency phonons have low scattering time implying they participate in scattering events more frequently. From the CDF and weighted CDF tables it is clear that the probability of being a transverse acoustic phonon is very high and hence their population is higher than the longitudinal phonons at TA phonon frequencies. This is also evident from polarization table plots shown in Fig. 3.14 and Fig. 3.15.
Figure 3.12: CDF Comparison Calculated from Different Approaches at 300K

Figure 3.13: Weighted CDF Comparison Calculated from Different Approaches at 300K
Figure 3.14: Polarization Table Comparison Calculated from Different Approaches at 300K

Figure 3.15: Weighted Polarization Table Comparison Calculated from Different Approaches at 300K
Figure 3.16: Scattering Times Comparison Calculated from Different Approaches at 300K
The thermal conductivity results for silicon is calculated through different approaches. Table 3.6 lists all the thermal conductivity calculation methods. The thermal conductivity of silicon calculated through the methods listed in Table 3.6 is as shown in Fig. 3.17, Fig. 3.18 and Fig. 3.19. It is evident that Mazumder’s way of simulating scattering event with Holland scattering rate and Lacroix’s way of simulating scattering event with calibrated Holland scattering rate are the best fits explaining the bulk thermal conductivity of silicon.
Figure 3.17: Thermal Conductivity of Silicon Calculated Through Mazumder’s Method

Figure 3.18: Thermal Conductivity of Silicon Calculated Through Lacroix’s Method
Mazumder’s approach of scattering gives incorrect temporal thermal profile. The temporal thermal profiles for different methods with Holland’s scattering rates at 300K are as shown in Fig 3.20, Fig 3.20, Fig 3.20. They clearly show that Mazumder’s approach of simulating the scattering event is not good. Lacroix’s method is good but the predicted thermal conductivity is not close to the experimental data. Calibrated Holland scattering rates produce closer match with Lacroix’s approach of simulating scattering event.
Figure 3.20: Transient Behavior of Temperature Profile Through Mazumder’s Approach Simulated with Holland Scattering Rates

Figure 3.21: Transient Behavior of Temperature Profile Through Lacroix’s Approach Simulated with Holland Scattering Rates
Figure 3.22: Transient Behavior of Temperature Profile Through Lacroix’s Approach Simulated with Calibrated Holland Scattering Rates
Chapter 4

CONCLUSIONS AND FUTURE WORK

A new way of modeling self-heating in nano-scale devices using multi-scale electro-thermal device simulation is presented. The solver is applied on understanding of self-heating effects in 22 nm planar MOSFET devices from IMEC. It is important to note that the electron problem is limited to length scales that are on the order of several tenths of nanometers. On the other hand, the phonon mean free path in bulk Si is on the order of 300 nm at room temperature, which is a much larger length scale. Hence, simulations of lattice heating require much larger simulation domain. In addition to this, as semiconductor device scaling progresses towards smaller dimensions, the role of interconnect self-heating has to be accounted for as well. For this purpose another level of hierarchy in the multi-scale modeling approach is introduced. Giga 3D (Silvaco Atlas module) is used to model the role of interconnects and the role of the larger simulation domain and is also used to extract the temperature boundary conditions for smaller domain electro-thermal device simulator. The electro-thermal simulator passes a Joule heating terms to Giga 3D and the whole Gummel iteration loop is repeated until a self-consistent solution at multiple levels of approximation is achieved.

To further improve the model accuracy, the Phonon Monte Carlo based thermal solver is introduced for electro-thermal device simulation. The PMC solver is tested and validated to explain the bulk thermal conductivity of silicon at different temperature. Comprehensive discussion on different PMC approaches in the literature is presented. Mazumder’s approach gives good match for the thermal conductivity, but the temporal temperature profile is incorrect. The reason is that Mazumder’s
approach assumes a Bose Einstein equilibrium distribution for the phonons at the end of each scattering event by choosing \( \delta t > 3 \tau_{\text{max}} \). However the spectrum of scattering rates shows that a single \( \delta t \) can not be chosen to fit all the phonons. This is partly avoided in Lacroix’s approach where the sampling after the scattering event is done from the modulated equilibrium distribution with probability of scattering. This improves the temporal temperature profile but the thermal conductivity is not matched with experimental data. To match with experimental thermal conductivity data, the scattering rates are calibrated. After calibration, the experimental data is closely matched with the predicted values.

The calibration is not required for calculating the thermal conductivity of silicon through direct solution methods for the phonon BTE. This shows that modeling the scattering events in the present approaches are not good enough to explain the thermal conductivity and necessary work has to be done to improve it. One way to improve is to simulate the scattering with energy and net momentum conservation following the full dispersion relation of phonons in silicon. This eliminates the need for sampling the phonons after scattering. This is computationally very expensive and requires more phonons to sample the k-space. Another way to improve is to follow relaxation time statistics without having to ignore any exponential terms in Eq. (3.48). These improvement will be done in the future work.

In the future, electro-thermal device simulator can be extended as depicted in Fig. 4.1. This will involve first, use of the thermal conductivity data that are calculated using LAMMPS simulation software in the original electro-thermal device simulator. Second, the energy balance solver will be replaced with a phonon Boltzmann transport solver that is already completed in the present work. LAMMPS simulation software will be used to calculate the proper phonon bandstructure that is input to the phonon Boltzmann transport equation solver.
Figure 4.1: Proposed Work for Future
REFERENCES


APPENDIX A

PLOTS FOR DATA CALCULATED FROM PRESENT WORK

In this appendix, the results of scattering table plots at 100K and 900K are presented. The cumulative distribution tables calculated from different approaches at 100K and 900K are as shown in Fig. A.1 and Fig. A.2 respectively.

![CDF tables comparison at 100K](image1)

Figure A.1: CDF Comparison Calculated from Different Approaches at 100K

![CDF tables comparison at 900K](image2)

Figure A.2: CDF Comparison Calculated from Different Approaches at 900K
The weighted CDF tables at 100K and 900K are as shown in Fig. A.3 and Fig. A.4 respectively. The scattering time comparison calculated from different approaches at 100K and 900K are as shown in Fig. A.5 and Fig. A.6 respectively.

Figure A.3: Weighted CDF Comparison Calculated from Different Approaches at 100K

Figure A.4: Weighted CDF Comparison Calculated from Different Approaches at 900K
Figure A.5: Scattering Times Comparison Calculated from Different Approaches at 100K
Figure A.6: Scattering Times Comparison Calculated from Different Approaches at 900K
The scattering time comparison calculated from different approaches at 100K and 900K are as shown in Fig. A.7 and Fig. A.8 respectively. The scattering time comparison calculated from different approaches at 100K and 900K are as shown in Fig. A.7 and Fig. A.8 respectively. These table plots are presented as reference for comparison with other similar works in phonon Monte Carlo studies.
Figure A.9: Weighted Polarization Table Comparison Calculated from Different Approaches at 100K

Figure A.10: Weighted Polarization Table Comparison Calculated from Different Approaches at 900K