The Phonon Monte Carlo Simulation

by

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A Thesis Presented in Partial Fulfilment
of the Requirements for the Degree
Master of Science

Approved November 2015 by the
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December 2015

ABSTRACT

Thermal effects in nano-scaled devices were reviewed and modeling methodologies to deal with this issue were discussed. The phonon energy balance equations model, being one of the important previous works regarding the modeling of heating effects in nano-scale devices, was derived. Then, detailed description was given on the Monte Carlo (MC) solution of the phonon Boltzmann Transport Equation. The phonon MC solver was developed next as part of this thesis. Simulation results of the thermal conductivity in bulk Si show good agreement with theoretical/experimental values from literature.

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Chapter 1

Introduction

As semiconductor devices are scaled down toward 10 nm regime, serious reliability issues appear as the heat generation and the elevated chip temperature cause undesirable effects in the integrated circuits. The hot-spot formed in the active region in a device is caused by the accumulated heat due to charge transport in the lattice and impedes the current flow. This self-heating effect occurs when the electrons accelerated by the electric field interact with the lattice vibration, i.e., the phonons in such a case when the device operates at the length scales comparable to both the electron and phonon mean free paths (approximately 5-10 nm for the electrons and 200-300 nm in bulk silicon for phonons at room temperature). The thermal conductivity of the semiconductor films thinner than the phonon mean free path is significantly reduced by phonon confinement and boundary scattering, which leads to a higher thermal resistance of a device and higher operating temperatures.

There are two ways to achieve improved device performance: use of alternative materials, such as strained Si and SiGe, and use of alternative devices such as silicon on insulator (SOI) technology (thin film transistors). The thin film SOI devices have great advantages of higher switching speeds and better turn-on characteristics over the bulk Si transistors. However, the thermal conductivity of the active device region is much lower than that of the bulk device, and strongly affected by phonon boundary scattering. Also, the thermal conductivity of the buried oxide layer is much lower than that of the active silicon region; hence it significantly impedes heat transfer through the substrate (large thermal resistance). Figure 1 shows thermal effects schematically in a silicon on insulator

(SOI) device and Table 1 shows that the thermal conductivities of 10 nm silicon and bulk SiO₂ are almost 1/10 and 1/100 times less than that of bulk silicon, respectively. The thermal conductivity observed and measured in single crystalline Si nanowires is also significantly lower than that of bulk Si, which suggests that phonon-boundary scattering controls thermal transport in Si nanowires. [1]

Figure 1: Hot spot caused by the electron-phonon interaction in a SOI device.

Table 1: Thermal Conductivities of some relevant materials used in device fabrication. [2]

Material	Thermal (W/mK)	Conductivity
Si (Bulk)	148	
Ge (Bulk)	60	
Silicides	40	
Si (10nm)	13	
SiO ₂	1.4	

Modeling thermal conductivity to understand the heat transport in semiconductor devices requires knowledge of how the lattice heat of the phonon system is distributed

Figure 2: Room temperature thermal conductivity data and predictions for thin Si films. [19]

throughout the collision process. Phonon transport in Si, for example, can be modeled using semi-classical methods because the phonon wave lengths dominating the heat conduction are approximately 1-2 nm, while the lattice constant a_0 is 0.5 nm. Semi-classical modeling includes the solution of the phonon Boltzmann transport equation (BTE), or the Monte Carlo technique for statistical simulation. The classical method of molecular dynamics, which does not involve the BTE solution, can also be used to calculate the critical parameters which can be applied to the BTE.

The evolution equation of a particle distribution function is called Boltzmann transport equation, and the exact solution of BTEs of the coupled electron and phonon systems is quite expensive. Although well-established techniques for the solution of the electron BTE exist, the BTE for phonons can be made soluble if the relaxation time approximation is involved. For common semiconductor materials, such as Si, Ge, and GaAs, the relaxation time approximation allows us to calculate the thermal conductivities in good agreement with the experimental data. The resolutions of the BTE for these materials in bulk state, thin film, or superlattice, have been achieved and the resolution based on the discrete

ordinates method or on the finite volumes method showed quick numerical convergence. However, they are governed by a single relaxation time taking into account all the different relaxation processes such as the anharmonic interaction of phonons, scattering with impurities and dislocation, or the boundary scattering.

On the other hand, the Monte Carlo (MC) method is a statistical sampling technique, which is quite plausible to solve the BTE because it can treat different scattering mechanisms separately, particularly for nontrivial geometries. The sole requirement of the method is to describe the process in terms of the probability density functions. The Ensemble Monte Carlo (EMC) method for electron has been developed in many studies. For example, in recent years Vasileska *et al.* have successfully investigated how the self-heating effect affect the electrical characteristics of the nano-scaled devices by implementing EMC simulator of electrons coupled with energy balance equation solver for the phonon bath [2].

While the transport of electrons has been solved by EMC method with great success, only a few studies have been performed the same for phonons. The difficulty of using MC to simulate the phonons comes from the fact that the number of phonons is not conserved in the system. Also, the phonons are not in an equilibrium distribution, there is no thermodynamic temperature to be dealt with in the relaxation time approximation. Still, the power of MC method is quite attractive and many attempts in the past have been made to solve the phonon BTE. For example, Mazumder and Majumdar obtained the steady-state phonon MC simulation results with the use of analytical phonon dispersion and using both acoustic polarization branches, but they did not present the transient regime [3]. In addition, the U and the N phonon processes were not treated separately. Later, Lacroix *et al.* included

those contributions and studied the influence of thermal conductivity dependence on heat conduction within a slab [4].

The molecular dynamics (MD) involves statistical mechanics to compute the transport coefficients, which can be used to calculate physical parameters for the BTE. Two major branches of the heat transport of MD simulations are the calculation of the thermal conductivity and the calculation of the phonon relaxation time. Those phonon relaxation times can then be used in the phonon energy balance solver.

In this report, the BTE for phonons and the derivation of the corresponding energy balance model is first reviewed. The EMC method for the electrons coupled with Poisson solver and energy balance equation for phonons is summarized and the simulation results are explained. Finally, the Monte Carlo solution of the phonon BTE is presented in details and representative simulation results are given to illustrate the validity of the approach.

Chapter 2

Modeling of Heat Transport

The thermal transport in a semiconductor device is combined with the charge transport through electron–phonon interaction. Modeling of the electron charge transport within the semi-classical framework includes the drift-diffusion model, the hydrodynamic model, and the EMC device simulation. Whatever the charge transport model is, the interaction of the electrons and the lattice of the crystal should be taken into account to complete the thermal transport since the electrons scattered by the lattice transfer the energy to the system.

The heat conduction equation is composed of energy conservation law and Fourier law.

The heat current carried by phonons under thermal gradient is given by

$$J_Q = \frac{1}{V} E_p N_k v_p = -\kappa \nabla T \quad (1)$$

where V is the volume, E_p is phonon energy, N_k is phonon distribution, v_p is phonon velocity, κ is thermal conductivity, and T is the temperature. The phonon distribution N_k should be properly dealt with to get the appropriate thermal conductivity. In order to understand the distribution function, let us consider the evolution of a general distribution function $f(\mathbf{r}, \mathbf{k}, t)$ which describes the number of particles depending on time t , location $\mathbf{r}$, and wave vector $\mathbf{k}$. This can also be defined as the mean particle number at time t in the volume $d^3\mathbf{r}d^3\mathbf{k}$ around the point $(\mathbf{r}, \mathbf{k})$ in the phase space. The time evolution equation of $f(\mathbf{r}, \mathbf{k}, t)$, which is called the Boltzmann transport equation (BTE), consists of diffusion of the particles, force exerted on the particles by the external influence, and collision of the particles as

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial t}\Big|_{\text{diffusion}} + \frac{\partial f}{\partial t}\Big|_{\text{force}} + \frac{\partial f}{\partial t}\Big|_{\text{collision}}, \quad (2)$$

or can be expressed as below:

$$\left(\frac{\partial}{\partial t} + \frac{\partial \mathbf{r}}{\partial t} \cdot \nabla_{\mathbf{r}} + \frac{\partial \mathbf{k}}{\partial t} \cdot \nabla_{\mathbf{k}} \right) f = \frac{\partial f}{\partial t}\Big|_{\text{collision}}. \quad (3)$$

If there is no external force, and using the fact that phonons have zero charge state, the BTE can be written as

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f = \frac{\partial f}{\partial t}\Big|_{\text{collision}} \quad (4)$$

where we can see that the key point in the BTE solution is modeling the collision term in the right hand side. Many studies approximate the collision term in the BTE by relaxation time approximation (RTA), where it is critical to calculate a suitable relaxation time τ .

Under the relaxation time approximation, the phonon BTE can be rewritten as

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f = -\frac{f - \bar{f}}{\tau} \quad (5)$$

where $\bar{f}$ is the Plank distribution at the local temperature.

Klemens [5], Callaway [6] and Holland [7] developed semi-empirical expressions for the relaxation rates that have allowed modeling of the thermal conductivity over a wide range of temperatures. However, those calculations should be corrected to adopt a realistic nonlinear phonon dispersion relationships.

A simpler way to capture the heat transfer from the electrons to the phonons can be accomplished by coupling the BTE for the electrons with the energy balance equations for the optical and acoustic phonon energy transfer, which can be derived from the phonon BTE. Let us consider how the energy of electrons and phonons is balanced in semiconductor material. For relatively low and moderate electric fields, the electrons

mainly interact with acoustic phonons. Under high electric field, $|\mathcal{E}| \geq 10^6$ V/m, which is characteristic for submicron semiconductor devices, the electrons get high energy enough to interact with optical phonons. This makes the lattice temperature influence the device current and other electrical characteristics. The most proper way to treat the self-heating problem without any approximation is to solve the coupled BTEs for electron and phonon system together. The heat transport described above tells us that the BTE for the two kinds of phonons (optical and acoustic modes) should be used to provide the energy balance of the process. The coupled system of semi-classical BTEs for the distribution functions of electrons $f(\mathbf{r}, \mathbf{k}, t)$ and phonons $g(\mathbf{r}, \mathbf{q}, t)$ in general are

$$\begin{aligned} \left(\frac{\partial}{\partial t} + \mathbf{v}_e(k) \cdot \nabla_r + \frac{e}{\hbar} E(r) \cdot \nabla_k \right) f \\ = \sum_q (W_{e,q}^{k+q \rightarrow k} + W_{a,-q}^{k+q \rightarrow k} - W_{e,-q}^{k \rightarrow k+q} - W_{a,q}^{k \rightarrow k+q}) \end{aligned} \quad (6)$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_p(q) \cdot \nabla_r \right) g = \sum_k (W_{e,q}^{k+q \rightarrow k} - W_{a,q}^{k \rightarrow k+q}) + \left(\frac{\partial g}{\partial t} \right)_{p-p} \quad (7)$$

In these expressions, $W_{e,q}^{k+q \rightarrow k}$ is the probability for electron transition from $k + q$ to k due to the emission of phonon q , and $W_{a,q}^{k \rightarrow k+q}$ refers to the process of absorption. However, these equations are non-linear and extremely difficult to solve. While the electron BTE has been dealt with EMC method by many studies, the complicated phonon BTE can be dealt by the energy balance equations to simulate the sub-micron semiconductor devices as long as the electron transport can be expressed with valid electron average velocity and effective electron temperature [8].

The energy balance equations are derived from the BTE through zeroth-, first-, and second-order moments to get carrier density, momentum, and energy conservation respectively as below:

$$\frac{\partial n}{\partial t} + \nabla \cdot n \mathbf{v}_e = \left. \frac{\partial n}{\partial t} \right|_c \quad (8)$$

$$\frac{\partial \mathbf{p}}{\partial t} + \nabla \cdot (v_e \mathbf{p}) = -en\mathcal{E} - \nabla(nk_B T_e) + \left. \frac{\partial \mathbf{p}}{\partial t} \right|_c \quad (9)$$

$$\frac{\partial u_e}{\partial t} + \nabla \cdot (\mathbf{v}_e u_e) = -en\mathbf{v}_e \cdot \mathcal{E} - \nabla \cdot (\mathbf{v}_e n k_B T_e) - \nabla \cdot \mathbf{J}_Q + \left. \frac{\partial u_e}{\partial t} \right|_c \quad (10)$$

where n is the electron number density, T_e is electron temperature. The electron momentum density $\mathbf{p}$ and energy density u_e can be written as

$$\mathbf{p} = m^* n \mathbf{v}_e \quad (11)$$

$$u_e = \frac{1}{2} (3n k_B T_e + m^* n v_e^2). \quad (12)$$

All the last terms with the subscript c indicate quantities due to collision events. The heat flux $\mathbf{J}_Q$ can be found from solving higher order moments of the BTE. In order to have a closed set of equations, it can be approximated as

$$\mathbf{J}_Q = -\kappa_e \nabla T_e, \quad (13)$$

where κ_e is the electron thermal conductivity.

The energy conservation equations for phonons are developed as follows. The phonon distribution function $N_k(x, t)$ can be expressed as

$$N_k(x, t) = \langle N_k \rangle_0 + n_k(x, t) \quad (14)$$

where $\langle N_k \rangle_0$ is the equilibrium phonon distribution at temperature T_e and $n_k(x, t)$ is the deviation of the phonon distribution function from equilibrium. Some other quantities are defined as sum of Eigen components as follows:

$$u(x, t) = \frac{1}{V} \sum_k n_k(x, t) \hbar \omega \quad (15)$$

$$\mathbf{S}(x, t) = \frac{1}{V} \sum_k n_k(x, t) \hbar \omega \mathbf{v}_k \quad (16)$$

$$\mathbf{J}(x, t) = \frac{1}{V} \sum_k n_k(x, t) \hbar \mathbf{k} \quad (17)$$

$$t^{ij}(x, t) = \frac{1}{V} \sum_k n_k(x, t) \hbar k^i v_k^j \quad (18)$$

where $u(x, t)$ is the energy density, $\mathbf{S}(x, t)$ is the energy flux, $\mathbf{J}(x, t)$ is the momentum density, $t^{ij}(x, t)$ is the momentum flux and $\mathbf{v}_k = d\omega/d\mathbf{k}$.

The collision of phonons with each other and imperfections causes every Eigen component except $\langle n_k \rangle_0$ to decay to zero with its own characteristic relaxation time. In order to apply the relaxation time approximation, a single relaxation time τ is used to characterize the decay to local equilibrium. This can be expressed as

$$\frac{\partial n_k(x, t)}{\partial t} + \mathbf{v}_k \cdot \nabla n_k(x, t) = - \frac{n_k(x, t) - n_k^0(T(x, t))}{\tau} \quad (19)$$

where $n_k^0(T(x, t))$ is the local equilibrium distribution and the value of $T(x, t)$ is determined according to energy conservation. The phonon energy balance equation is obtained by multiplying phonon BTE with RTA, Eq. (19), by $\hbar \omega_k$ and then summing over all modes as

$$\frac{1}{V} \sum_k \hbar \omega_k \frac{\partial n_k(x,t)}{\partial t} + \frac{1}{V} \sum_k \hbar \omega_k \mathbf{v}_k \cdot \nabla n_k(x,t) = -\frac{1}{V} \sum_k \hbar \omega_k \frac{n_k(x,t) - n_k^0(T(x,t))}{\tau} \quad (20)$$

$$\begin{array}{ccc} \Downarrow & \Downarrow & \Downarrow \\ \frac{\partial u(x,t)}{\partial t} & \nabla \cdot \mathbf{S}(x,t) & 0 \end{array}$$

Therefore we have the reduced form of Eq. (20) as

$$\frac{\partial u(x,t)}{\partial t} + \nabla \cdot \mathbf{S}(x,t) = 0 \quad (21)$$

Then again multiplying Eq. (20) with $\hbar \omega_k v_k^i$ where $i = x, y, z$ and summing over all modes gives

$$\begin{aligned} \frac{1}{V} \sum_k \hbar \omega_k v_k^i \frac{\partial n_k(x,t)}{\partial t} + \frac{1}{V} \sum_k \hbar \omega_k v_k^i \mathbf{v}_k \cdot \nabla n_k(x,t) \\ = -\frac{1}{V} \sum_k \hbar \omega_k v_k^i \frac{n_k(x,t)}{\tau} \end{aligned} \quad (22)$$

which reduces to

$$\frac{\partial \mathbf{S}_i(x,t)}{\partial t} + \frac{1}{V} \sum_j \sum_k \hbar \omega_k v_k^i v_k^j \frac{\partial n_k(x,t)}{\partial X_j} = -\frac{\mathbf{S}_i(x,t)}{\tau}. \quad (23)$$

Introducing the temperature gradient on the second term in the left hand side of Eq. (23) as

$$\frac{\partial n_k(x,t)}{\partial X_j} = \frac{\partial n_k(x,t)}{\partial T} \frac{\partial T}{\partial X_j} \quad (24)$$

we can arrive

$$\left(\tau \frac{\partial}{\partial t} + 1 \right) \mathbf{S}_i(x,t) = -\frac{\tau}{V} \sum_j \sum_k \hbar \omega_k v_k^i v_k^j \frac{\partial n_k(x,t)}{\partial T} \frac{\partial T}{\partial X_j}. \quad (25)$$

Let us define κ_{ij} as the thermal conductivity tensor by

$$\kappa_{ij} = \frac{\tau}{V} \sum_j \sum_k \hbar \omega_k v_k^i v_k^j \frac{\partial n_k(x,t)}{\partial T} \quad (26)$$

Then Eq. (25) can be expressed as

$$\left(\tau \frac{\partial}{\partial t} + 1\right) \mathbf{S}(x, t) = -\kappa \nabla T. \quad (27)$$

Applying divergence on both sides of the above equation results

$$\left(\tau \frac{\partial}{\partial t} + 1\right) \nabla \cdot \mathbf{S}(x, t) = -\nabla \cdot \kappa \nabla T. \quad (28)$$

From Eq. (21),

$$\nabla \cdot \mathbf{S}(x, t) = -\frac{\partial u(x, t)}{\partial t}, \quad (29)$$

and since $u(x, t)$ can be expressed with heat capacity C_0 we have

$$u(x, t) = C_0 [T_0 - T(x, t)]. \quad (30)$$

Then, Eq. (28) becomes

$$C_0 \left(\tau \frac{\partial}{\partial t} + 1\right) \frac{\partial T(x, t)}{\partial t} = -\nabla \cdot \kappa \nabla T + H \quad (31)$$

where the first term on the right hand side means the influx of energy into a volume dV and the second term H , which comes from the time evolution of $C_0 T_0$, denotes the increase in the energy due to electron-phonon interaction in the system. Also, the relaxation time dependent term in the left hand side can be negligible, we have the final form of

$$C_0 \frac{\partial T(x, t)}{\partial t} = -\nabla \cdot \kappa \nabla T + H. \quad (32)$$

The process in which the energy exchange takes place between the electrons and phonons differs depending on how the particle scattering occurs. Therefore the energy balance equations are derived separately for acoustic phonons and optical phonons. As the primary path of energy transport is represented first by scattering between the electrons at T_e and optical phonons at T_{Lo} and then optical phonons decaying to acoustic phonons at T_A

to the lattice at T_L , which is estimated as equivalent to T_A . The energy exchange between the electrons and the phonons comes from Eq. (12) to electron-optical energy balance as following

$$C_{LO} \frac{\partial T_{LO}}{\partial t} = -\nabla \cdot \kappa_{LO} \nabla T_{LO} + \frac{1}{2} \frac{[3nk_B(T_e - T_{LO}) + m^* n v_e^2]}{\tau_{e-LO}} - C_{LO} \frac{T_{LO} - T_A}{\tau_{LO-A}}. \quad (33)$$

The first term in the right hand side goes to 0 because the group velocity of optical phonon is near 0. The second term represents the energy gain from the electrons, and the last term is the energy loss to the acoustic phonons. So the final form is given by

$$C_{LO} \frac{\partial T_{LO}}{\partial t} = \frac{1}{2} \frac{[3nk_B(T_e - T_{LO}) + m^* n v_e^2]}{\tau_{e-LO}} - C_{LO} \frac{T_{LO} - T_A}{\tau_{LO-A}} \quad (34)$$

The next step of optical-acoustic phonon energy balance is shown as

$$C_A \frac{\partial T_A}{\partial t} = -\nabla \cdot \kappa_A \nabla T_A + \frac{3nk_B(T_e - T_L)}{2\tau_{e-L}} + C_{LO} \frac{T_{LO} - T_A}{\tau_{LO-A}} \quad (35)$$

where we do not have electron velocity related term in the second of the right hand side of course, and if the electron-acoustic phonon scattering is elastic, the whole second term should be excluded. The last term indicates the energy gain from optical phonons coming from the last term of the right hand side of Eq. (34).

Chapter 3

Solution of the Phonon BTE - Previous Works

Mostly, the previous work performed and related to thermal modeling can be split into (1) the solutions of the phonon BTE or (2) the analysis of self-heating effects in devices. One of the initial solutions of phonon BTE was done by Peterson, who performed a Monte Carlo Simulation for phonons in the Debye approximation using single relaxation time [9]. Mazumder and Majumdar followed Peterson's approach including the dispersion relation and the different acoustic polarization branches [3]. However, the N and the U processes were not treated separately although they do not contribute the same way to the thermal conductivity. Lacroix further generalized the model by incorporation of N and U processes, and the transient conditions were considered as well [4]. Figure 3 and Figure 4 show the phonon MC simulation results for Germanium.

Figure 3: Transient temperature in Fourier's regime for germanium and comparison with the analytical solution of heat conduction equation with a constant thermal diffusivity. [4]

Figure 4: Silicon and germanium thermal conductivities calculated by MC method.

On the other hand, Eric Pop [10], Goodson [11], and Robert Dutton [12] worked on modeling self-heating in devices. They used non-parabolic band model for the electrons combined with analytical phonon dispersion and studied heat transfer and energy conversion processes at the nanoscales. Applications included semiconductor devices and packaging, thermoelectric and photonic energy conversion, and microfluidic heat exchangers.

One of the recognizable works of modeling thermal effect in devices is done by Raleva and Vasileska [2]. The simulator developed by this group is based on EMC method to solve electron BTE self-consistently with energy balance equations for phonon transport. That has been applied to the FD SOI devices showing that the velocity overshoot takes place in the nano-scaled devices and minimizes the degradation of the device characteristics due to lattice heating because of ballistic transport effects. This simulator has been proved to be successful to describe impact of self-heating effects in SOI devices down to 25nm channel length. Figure 6 shows how the simulator works and Figure 5

demonstrates I-V characteristics of the device. The plot in Figure 7 illustrates the lattice temperature distribution in the Si layer when the gate temperature is assumed to be 300K. As the gate size gets smaller, the hot spot moves toward the drain and this behavior is less pronounced when the gate temperature is higher.

Figure 5: Left panel: Output characteristics for $V_{gs}=1.2$ V Right panel: Velocity along the channel for $V_{gs}=1.2$ V and different values for V_{ds} . [2]

Figure 6: Left panel: Exchange of variables between the two kernels. Right panel: Choice of the proper scattering table. [2]

As the scale goes down below 20nm regime, however, quantization effect starts to play a significant role, and the semiclassical transport description for the electrons would be no longer valid. In order to explain the self-heating effects in those ultra-short channel devices, whose dimension is comparable to the mean free path of the electrons, the proper quantum transport description for the electrons is essential. On the other hand, even for those ultra-short channel devices, the heat transfer would be treated within the limits of the validity of the semi-classical transport theory by solving BTE for phonon with the relaxation time approximation, though the multiple phonon modes should be included to have more

Figure 7: Lattice temperature profiles in the Si layer with gate temperature of 300K (left) and 400K (right). [2]

accurate model. Adopting Monte Carlo simulation of phonon system makes it possible to track each scattering mechanism independently regardless of the geometry, and has the main advantage of the simple treatment of transient problems without actually solving the exact BTE.

This work will present the phonon MC simulator, which will be coupled with the device simulator for the electrons to model thermal effects in nano-scaled devices such as nano-wires, ultra-short channel SOI devices, and FinFET in future works. The first step in developing global BTE solver for both electrons and phonons is the development of a phonon MC simulator.

Chapter 4

Phonon Monte Carlo Simulation

4.1 Theory for the Lattice Modeling [13] [14] [15] [16]

The concept of phonon is introduced as quantized elastic waves. The atoms at the lattice sites of a dielectric crystal experience small oscillations about their equilibrium positions at any temperature. The heat conduction is described in terms of the energy of lattice vibrations called phonons. This particle description is quite useful in treating interactions with electrons. The crystal Hamiltonian H is represented as:

$$H = H_l + H_e, \quad (36)$$

with the lattice Hamiltonian H_l of the lattice kinetic energy and the interionic potential as

$$H_l = \sum_l \frac{p_l^2}{2M_l} + \sum_l \sum_{m \neq l} U(\mathbf{R}_l - \mathbf{R}_m), \quad (37)$$

where M is phonon mass, U is phonon potential, $\mathbf{R}$ is real position of phonon, and the electron Hamiltonian H_e of the electron kinetic energy and electron-electron, electron-ion interaction as

$$H_e = \sum_i \frac{p_i^2}{2m_i} + \sum_i \sum_j \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} + \sum_i \sum_l V(\mathbf{r}_i - \mathbf{R}_l). \quad (38)$$

The first approximation for the whole Hamiltonian is that only the valance electrons can be dealt while the core being left alone. The second approximation, so called adiabatic approximation, comes from the fact that the ions are much heavier than the electrons, so ions are relatively stationary for electrons, and only a time-averaged electronic potential is seen for ions. In other words, the whole Hamiltonian can be separated into the part of electrons and that of phonons. As that being said, the first and second term of Eq.(38) gives

us the information of energy band diagram of the material, and Eq.(37) gives the dispersion relation of phonons.

For the lattice Hamiltonian, as we describe the lattice vibration as an oscillator, we have

$$H_l \phi_l = E_l \phi_l, \quad \phi_l \Rightarrow |n_{q1} n_{q2} n_{q3} \dots \dots \rangle \quad (39)$$

$$E_l = \sum_q \hbar \omega \left(\langle n_q \rangle + \frac{1}{2} \right) \quad (40)$$

when the mode is excited to quantum number n_q : that is, when the mode is occupied by n_q phonons. This n_q is determined by Bose-Einstein distribution as

$$\langle n_q \rangle = \frac{1}{\exp(\hbar \omega / k_B T) - 1}. \quad (41)$$

A phonon of wave vector q will interact with the particles such as phonons and electrons as if it had momentum $\hbar q$. However, $\hbar q$ is not actually a physical momentum but a crystal momentum because q is considered to have a smallest magnitude of $|q|$ in its family set of $\left(q \pm \frac{2\pi}{a}, q \pm \frac{4\pi}{a}, \dots \right)$, and so on. So the momentum of phonon is transferred to the lattice as a whole except for the case of uniform mode $q = 0$, when the whole lattice translates with the linear momentum.

The equation of motion of the phonons for the monatomic basis begins with the total force on the planes $s, s \pm 1$ with the displacement u :

$$F_s = C(u_{s+1} - u_s) - C(u_s - u_{s-1}). \quad (42)$$

The equation of the motion of the plane is then

$$M \frac{d^2 u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s), \quad (43)$$

where M is the atom mass. The solution of u_s has the time dependence in the form of $\exp(-i\omega t)$ as $d^2u_s/dt^2 = -\omega^2u_s$ and shows the periodicity as

$$u_{s+1} = u_s \exp(\pm iqa), \quad (44)$$

where a is the space between planes and q is the wave vector, and ω in terms of q is described as:

$$\omega^2 = \frac{2C}{M}(1 - \cos qa). \quad (45)$$

The equation that relates the frequency of a phonon, ω to its wave vector q is known as a dispersion relation which can be rewritten as

$$\omega = 2 \left(\frac{C}{M} \right)^{\frac{1}{2}} \left| \sin \left(\frac{qa}{2} \right) \right| \quad (46)$$

with the boundary condition of the first Brillouin zone at $q = \pm \pi/a$. The phonon dispersion relation of Si is shown in Figure 8.

The speed of propagation of a phonon, which is also the speed of the sound in the lattice, is given by the slope of the dispersion relation $\partial\omega/\partial q$ (the group velocity). At low values of q , the dispersion relation is almost linear and the speed of the sound becomes $\sqrt{C/M} a$, independent of the phonon frequencies.

For a crystal that has at least two atoms in a unit cell, the dispersion relation develop two types of phonons, namely, optical and acoustic modes corresponding to the upper and lower sets of the curves respectively. For the optical branch at $q = 0$ with two phonon displacement u and v , we find

$$\frac{u}{v} = -\frac{M_2}{M_1} \quad (47)$$

Figure 8: The phonon dispersion relation in Si along Γ to X point.

The atoms vibrate against each other (the neighboring atoms oscillate in the opposite direction), but their center of mass is fixed. For the acoustic branch the atoms and their center of mass move together in the same direction as in long wavelength acoustic vibration.

Phonons have multiple polarizations depending on whether the atomic displacement is perpendicular (transverse) or parallel (longitudinal) to the wave vector. If there are p atoms in the primitive cell, there are $3p$ branches to the dispersion relation: 3 (1 longitudinal + 2 transverse) acoustical and $(3p - 3)$ optical branches.

The electrons with low energy (< 50 meV) scatter mainly with acoustic phonons, while those with high energy scatter most effectively with optical modes [10]. The optical phonon modes have high energy with low group velocity (~ 1000 m/s) and relatively low occupancy, hence the heat transport is dominated by the acoustic phonon modes which are

Figure 9: Diagram and characteristic time scales of energy transfer processes in silicon. [2] significantly populated and have large group velocity ($\sim 5000 - 9000$ m/s). The optical phonons eventually decay into acoustic modes over longer period of time (picoseconds), while electron-optical phonon scattering relaxation time is on the order of 0.1 pico-seconds. Based on that, the primary path of energy transport is represented first by scattering between electrons and optical phonons and then optical phonons to the lattice. Since as much as $2/3$ amount of the thermal energy is initially stored in the optical phonon modes, this may create a phonon energy bottleneck until the optical phonons decay into the faster acoustic modes. This means that the density of the optical phonon modes build up over time elevating the temperature in the active region of the device and thus forming a hot-spot to cause more scattering mechanism to impede the carrier transport. That is shown in Figure 9.

The thermal conductivity coefficient κ is defined with respect to the flux of thermal energy j_U down a long rod with a temperature gradient dT/dx :

$$j_U = -\kappa \frac{dT}{dx}. \quad (48)$$

The thermal conductivity κ can be expressed as

$$\kappa = \frac{1}{3} C v l, \quad (49)$$

where C is the heat capacity, v is the average particle velocity, and l is the mean free path between collision. Since the velocity (of sound) is almost temperature independent, the thermal conductivity is determined by the heat capacity and the phonon mean free path. The phonon mean free path l is determined by (1) geometrical scattering, and (2) scattering by other phonons, all of which depend strongly on temperature. If the forces between atoms are purely harmonic, there would be no collision between phonons, and the mean free path would be limited by the phonon scattering with the crystal boundary and by the lattice imperfections. At very low temperature, phonon mean free path could be even larger than the structure length, boundary scattering does not play any role. The thermal conductivity κ is solely determined by heat capacity C and will go as T^3 . As the temperature increases, anharmonic U processes begin to appear and will gradually make the phonon mean free path smaller than the structure dimension. Thermal conductivity reaches its maximum at this point and then begins to fall exponentially as it is inversely proportional to the number of U processes as $e^{\hbar\omega/k_B T}$. At higher temperatures, the exponential fall is replaced by slow $1/T$. Anharmonic decay is caused by the cubic and higher terms of the crystal potential. The cubic term gives rise to the three-phonon process where a phonon breaks up or decays into two phonons while conserving total crystal energy and momentum. The first of the three phonons involved in the anharmonic process is given by the initial phonon wave vector $\mathbf{q}$. Then the second phonon wave vector $\mathbf{q}'$ is chosen uniformly at random from the

entire first Brillouin zone. Finally the third phonon is produced by momentum conservation as the difference between initial and the randomly chosen momenta $\mathbf{q}'' = \mathbf{q} - \mathbf{q}' + \mathbf{G}$, where $\mathbf{G}$ is a basis vector in reciprocal space ensuring that the resulting $\mathbf{q}''$ falls within the first Brillouin zone. For processes where all three vectors are contained in the first Brillouin zone, the value of $\mathbf{G}$ is zero and the process is called *Normal*. Normal process does not impede phonon momentum, therefore does not impede heat flow directly, but affect by re-distributing phonon energies. Those processes where one of the final momentum vectors lands outside of the first Brillouin zone have non-zero values of $\mathbf{G}$ and are called *Umklapp*. Such processes cause thermal resistivity and dominate the thermal conductivity, participating in the decay of intra-valley optical phonons. The phonon mean free path which enters Eq. (49) is the mean free path for Umklapp collision.

Callaway developed a phenomenological model for lattice thermal conductivity at low temperature by assuming that the phonon scattering processes can be represented by frequency-dependent relaxation time [6]. The combined relaxation time from BTE in the presence of temperature gradient is

$$\tau_c^{-1} = A\omega^4 + BT^3\omega^2 + c/L, \quad (50)$$

where $A\omega^4$ represents the scattering by point impurities, $BT^3\omega^2$ normal and Umklapp process, c/L boundary scattering, c is the velocity of sound and L is the characteristic length of the material. Then the thermal conductivity κ is found to be

$$\kappa = \frac{c^2}{2\pi^2} \int \tau_c \left(1 + \frac{\beta}{\tau_N}\right) C_{ph} k^2 dk, \quad (51)$$

where C_{ph} is the phonon specific heat. The combined relaxation time τ_c is multiplied by the factor $(1 + \beta/\tau_N)$, where β is the parameter defined by the dimensions of relaxation

time and τ_N is the relaxation time for normal process, which expresses the correction due to the distribution function change. Callaway's final formula shows that the thermal conductivity in the region just beyond the low-temperature maximum will be proportional to $T^{-2/3}$ for normal material and T^{-2} for isotopically pure material. At very low temperatures, κ is proportional to T^3 , which obeys Debye law.

Holland represented an analysis of lattice thermal conductivity which considers both longitudinal and transverse phonons using relaxation time approximation. The thermal conductivity of phonons with wave vector q and polarization s has the form of

$$\kappa = \frac{1}{(2\pi)^3} \sum_s \int v_{q,s}^2 \tau(\mathbf{q}, s) C_{ph}(\mathbf{q}, s) d\mathbf{q}. \quad (52)$$

The relaxation times consist of

$$\tau^{-1} = \tau_b^{-1} + \tau_I^{-1} + \tau_{ph-ph}^{-1}, \quad (53)$$

where τ_b^{-1} is the relaxation time for boundary scattering and has the form of v_s/LF , adding factor F for a correction. The relaxation time for impurity scattering τ_I^{-1} is of the form $A\omega^4$. The significant difference from Callaway's formula comes from the relaxation time for three phonon scattering τ_{ph-ph}^{-1} , where the longitudinal ($\propto \omega^2 T^3$ for low T , $\propto \omega^2 T$ for high T) and transverse ($\propto \omega T^4$ for low T , $\propto \omega T$ for high T) modes are distinguished. Figure 10 shows Holland's thermal conductivity model fitted to experimental data. His relaxation times have been adapted to this phonon MC simulation work, which will be explained in later part of this chapter.

Modeling thermal conductivity is quite complex and challenging because of the phonon mean free path depending on temperature and impurity concentration in integration of the

volume of the material as seen above. For known phonon mean free path of bulk material, the thermal conductivity can be modeled numerically as [17]

$$\kappa = \frac{1}{3} C v l \approx \frac{1}{3} \int_i C_\omega v_\omega \left(\frac{A_1}{D} + \frac{A_2}{l_0} + A_3 N_i \right)^{-1} d\omega, \quad (54)$$

where C_ω is the heat capacity per unit frequency mode, v_ω is the mode velocity, D is the diameter of nanowire, l_0 is the phonon mean free path in the bulk material, N_i is the impurity concentration, and A_1, A_2, A_3 are fitting parameters. The term in parenthesis represents the various contributions to the phonon mean free path, including boundary scattering which becomes the limiting term when the diameter D falls below the range of the bulk phonon mean free path (0.1-1 μ m). Variations on the expression above have generally been successful in reproducing experimental data on thermal conductivity of silicon.

Figure 10: Thermal conductivity of Si by Holland's formula with experimental data. [7]

Two types of intervalley scattering are possible in silicon; ‘g-type’ processes move a carrier from a given valley to one in the opposite side of the same axis. The ‘f-type’ processes move a carrier to one of the remaining valleys. Z. Aksamija et al. [18] showed that the most of the longitudinal optical (LO) g-type phonons decay into one longitudinal acoustic (LA) and one transverse acoustic (TA) phonon, and those LA phonons from anharmonic decay are non-equilibrium and have energies around 40meV. This leads to re-absorption of non-equilibrium phonons by the electrons and cause the hot electron effect and reliability problems.

Liu and Asheghi presented the thermal conduction in ultra-thin (30nm) pure and doped single crystal silicon layers at high temperature (300-450K) range [19]. They showed that the experimental thermal conductivity data can be interpreted using thermal conductivity integral in relaxation time approximation that accounts for phonon-boundary and phonon-impurity scatterings. According to the results, the thermal conductivities of Si layers are significantly lower than the values for bulk samples due to the much stronger reduction of

Figure 11: Thermal conductivities calculated using the complete dispersion relation for Si nanowires of diameters 38.85nm(solid), 72.8nm(dotted), and 132.25nm(dashed). Dots: experimental data from Li [21]

phonon mean free path by boundary scattering. The effect of phonon-boundary scattering is reduced at higher temperatures because of the smaller phonon mean free path in bulk silicon.

Mingo presented that it is possible to predictively calculate lattice thermal conductivity by using complete phonon dispersion for silicon nanowires wider than 35nm, for which phonon confinement effects are not important [20]. Figure 11 Shows that the theoretical model agrees well with the experimental data [21].

4.2 Simulation using Monte Carlo Method

Figure 12: Flowchart for phonon MC.

As it has been shown above, the crystal under thermal effect can be described by the phonon characteristics of location in real and momentum space, (group) velocity, and polarization, which can be obtained by solving BTE. The main advantages of adapting Monte Carlo method for that purpose are: simpler handling of transient problem without having to solve BTE directly, the capability of treating any geometries (such as transistor), and the ability to track each phonon with each scattering process. The phonon MC requires:

- modeling lattice,
- setup boundary conditions, and
- arranging scattering table.

The flowchart of phonon MC is shown in Figure 12.

4.3 Simulation Domain

MC technique is most competitive in case of nontrivial geometry. For any complex shape of material or device, the only thing we need to consider carefully is the boundary condition of the model. For the bulk simulation, a stack of 40 simple cubic cells is used as a medium and the temperature of both end walls are set to constants. Incoming phonons in these end cells are thermalized at each time step as if those are blackbodies. The three discretizations of spatial, spectral, and temporal are chosen. The spatial discretization is related to the geometry of the material, and the time step must be lower than $\Delta t < L_z/v_g^{\max}$, where L_z is the length of the unit cell, $v_g^{\max}$ is the maximum group velocity of phonon, so that all scattering mechanism can be considered and ballistic jumping over several cells can be avoided. $N_b = 1000$ spectral bins in the range $[0, \omega_{LA}^{\max}]$ is used for the spectral discretization.

4.4 Initialization of Phonons

The first step of the simulation, which is the initialization of the state of phonons requires the information of the number of phonons in each cell. This can be obtained by considering the local temperature and energy. The phonon wave vectors are assumed to be dense enough in $\mathbf{q}$ -space so that the summation over $\mathbf{q}$ can be replaced by an integral. Then the integration in the frequency domain can be achieved from Eq. (40) and Eq. (41) as

$$E = \sum_p \int_{\omega} \left(\langle n_{\omega,p} \rangle + \frac{1}{2} \right) \hbar \omega D_p(\omega) g_p d\omega \quad (55)$$

where g_p is the degeneracy of the branch and $D_p(\omega)d\omega$, the phonon density of state, describes the number of vibrational modes in the frequency range $[\omega, \omega + d\omega]$ for polarization p . For an isotropic three-dimensional crystal ($V = L^3$), the phonon density of states in $\mathbf{q}$ -space can be described as

$$D_p(\omega)d\omega = \frac{d\mathbf{q}}{(2\pi/L)^3} = \frac{V q^2 dq}{2\pi^2}. \quad (56)$$

The $1/2$ term in Eq. (55) indicates the constant zero point energy which is not the case for the energy transfer in the material, so it can be suppressed and the energy can be expressed as

$$E = V \sum_p \int_{\omega} \left[\frac{\hbar \omega}{\exp\left(\frac{\hbar \omega}{k_B T}\right) - 1} \right] \frac{q^2}{2\pi^2 v_g} g_p d\omega. \quad (57)$$

If we think of $E = N \hbar \omega$ then the number of phonons in each cell is obtained by combining Eq. (55) and Eq. (57) along with Eq. (41) as

$$N = V \sum_{p=\text{TA,LA}} \sum_{b=1}^{N_b} \left[\frac{1}{\exp\left(\frac{\hbar\omega_{b,p}}{k_B T}\right) - 1} \right] \frac{q_{b,p}^2}{2\pi^2 v_{gb,p}} g_p \Delta\omega \quad (58)$$

where TA and LA means the polarization of transverse acoustic and longitudinal acoustic, and $v_{gb,p}$ is the group velocity defined by $(\Delta\omega/\Delta q)$. N_b is chosen to be 1000 as the spectral discretization. This actual number in the order of ($\sim 10^{22}$ phonons/m³) is too large to handle, so the super particle N^* is introduced and defined with the weight factor W , which is used during the simulation as

$$N^* = \frac{N}{W} \quad (59)$$

so that we have N^* in the order of ($\sim 10^4$) for less expensive simulation.

The first cell is fixed to the hot temperature T_h and the end cell to the low temperature T_c . All the intermediate cells are also at T_c in the initialization process. The theoretical energy obtained from Eq. (57) should match the energy E^* calculated in all the cells as following:

$$E^* = \sum_{c=1}^{N_{\text{cell}}} \sum_{n=1}^{N^*} W \times \hbar\omega_{n,c}. \quad (60)$$

The phonons are randomly distributed within the limit as described above by the dispersion relation. The rule for how many phonons should be distributed along to the spectral discretization bin is governed by the normalized number density function F :

$$F_i(T) = \frac{\sum_{j=1}^i N_j(T)}{\sum_{j=1}^{N_b} N_j(T)} \quad (61)$$

The random number R is drawn. If $F_{i-1} \leq R \leq F_i$ then the location is achieved using bisection algorithm, and corresponding value F_i gives the frequency $\omega_{0,i}$, the central

frequency of the i th interval. The actual frequency of the phonon is randomly chosen in the spectral bin by

$$\omega_i = \omega_{0,i} + (2R - 1) \frac{\Delta\omega}{2}. \quad (62)$$

The polarization of phonon is determined by the probability to find a LA phonon P_{LA} as

$$P_{\text{LA}}(\omega_i) = \frac{N_{\text{LA}}(\omega_i)}{N_{\text{LA}}(\omega_i) + N_{\text{TA}}(\omega_i)}. \quad (63)$$

If a new random number $R < P_{\text{LA}}(\omega_i)$, the phonon belongs to the LA branch, otherwise it does to the TA branch. The number of phonons in each branch, $N_{\text{LA}}(\omega_i)$ and $N_{\text{TA}}(\omega_i)$ can be obtained by

$$N_{\text{LA}}(\omega_i) = \langle n_{\text{LA}}(\omega_i) \rangle D_{\text{LA}}(\omega_i), \quad (64)$$

$$N_{\text{TA}}(\omega_i) = 2 \times \langle n_{\text{TA}}(\omega_i) \rangle D_{\text{TA}}(\omega_i), \quad (65)$$

where the density function $D_{\text{LA}}(\omega_i)$ and $D_{\text{TA}}(\omega_i)$ are calculated using Eq.(56).

Once the frequency and the polarization are known, the group velocity and the wave vector can be determined by the dispersion relation. The whole phonon dispersion relation should be well taken into account for the realistic simulation of phonon transport through the crystal. Here for the MC simulation, however, the optical phonons are not considered because they have low group velocity and do not significantly contribute to the heat transfer even though they still can affect the total conductivity through the acoustic phonons by modifying the relaxation time. Therefore we have two polarization branches of TA (transverse acoustic) and LA (longitudinal acoustic). The numerical dispersion relation data was taken from the isotropic approximation by E. Pop [22] as

$$\omega_q = \omega_0 + v_s q + c q^2 \quad (66)$$

where the coefficients determined by fitting parameters can be found from Table 2.

Table 2: Quadratic phonon dispersion coefficients [22].

	ω_0 10^{13}rad/s	v_s 10^5cm/s	c $10^{-3}\text{cm}^2/\text{s}$
LA	0	9.01	-2.00
TA	0	5.23	-2.26

The group velocity can be extracted from the dispersion relation as

$$v_g = \frac{\partial \omega}{\partial q} = v_s + cq. \quad (67)$$

When we generate the dispersion relation for the simulation, first we get $v_{g, \max}$ at $q = 0$ using Eq. (67) for LA and TA branches, and then get $\omega_{\max}$ at $q_{\max} = 2\pi/a$ (where a is lattice constant) using Eq. (66). Now we can randomly distribute phonons in the cell according to the dispersion relation in the limit of $[0, q_{\max}]$ and $[\omega_{\min}, \omega_{\max}]$. The phonon dispersion relation simulated by this initialization step is shown in Figure 13.

The positions of the n th phonon in real space in the cell, whose lengths are L_x , L_y , and L_z is given by three random numbers as

Figure 13: Phonon dispersion curve for Si by the initialization step of MC simulation

$$\mathbf{r}_{n,c} = \mathbf{r}_c + L_x R \mathbf{i} + L_y R' \mathbf{j} + L_z R'' \mathbf{k}, \quad (68)$$

where $\mathbf{r}_c$ is the coordinate of the cell. The wave vector direction $\boldsymbol{\Omega}$ is obtained by two random numbers as

$$\boldsymbol{\Omega} = \begin{cases} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{cases} \quad (69)$$

where $\cos \theta = 2R - 1$ and $\phi = 2\pi R'$.

4.5 Diffusion

After the initialization, the phonons move and diffuse by the group velocity inside the cell, and some of them jump to the neighboring cell. The position of the phonon is updated as $\mathbf{r}_{\text{diff}} = \mathbf{r}_{\text{old}} + \mathbf{v}_g \Delta t$. At the end of the diffusion phase, the actual energy in the cell is calculated and based on this, the actual temperature is obtained. The phonons in both end cells of the stack are thermalized to the constant hot or cold temperature as if the cells act like blackbodies.

4.6 Scattering

The scattering process is treated independently from the diffusion. The most important scattering mechanism in the phonon system is three phonon process: normal process(N) preserves momentum and Umklapp(U) process does not. U process becomes significant and directly modify heat propagation when the temperature is high ($T \geq T_{\text{Debye}}$). N process also affects heat transfer because it changes the phonon frequency distribution. When the phonons $(p, \omega, \mathbf{q})$ and $(p', \omega', \mathbf{q}')$ scatter to $(p'', \omega'', \mathbf{q}'')$, three phonon scattering is expressed by

$$\begin{aligned}
&\text{energy: } \hbar\omega + \hbar\omega' \leftrightarrow \hbar\omega'', \\
&N \text{ process: } \mathbf{q} + \mathbf{q}' \leftrightarrow \mathbf{q}'', \\
&U \text{ process: } \mathbf{q} + \mathbf{q}' \leftrightarrow \mathbf{q}'' + \mathbf{G}
\end{aligned} \tag{70}$$

where $\mathbf{G}$ is a lattice reciprocal vector.

In this phonon MC simulation, the phonon collision process is treated in the relaxation time approximation. The relaxation times of N and U processes for the LA and TA branches are taken from Holland's work on Si [7]. The probability for a phonon to be scattered during Δt is

$$P_{\text{scat}} = 1 - \exp\left(\frac{-\Delta t}{\tau_{NU}}\right) \tag{71}$$

where τ_{NU} is a global three-phonon relaxation time accounting for N and U processes. If a random number $R \geq P_{\text{scat}}$ then the phonon is self-scattering. When we have a N process scattering rate $\Gamma_N = \tau_N^{-1}$ and a U process scattering rate $\Gamma_U = \tau_U^{-1}$, $\Gamma_{NU} = \Gamma_N + \Gamma_U$ and for $R \leq \Gamma_N/\Gamma_{NU}$ the phonon has normal process. τ_{NU} is obtained by Mathiessen rule ($\tau_{NU}^{-1} = \tau_N^{-1} + \tau_U^{-1}$). For the TA branch, there is a frequency limit and ω_{limit} corresponds to the frequency when $\mathbf{q} = \mathbf{q}_{\text{max}}/2$ from where phonon frequency becomes independent of wave vectors. If $\omega \leq \omega_{\text{limit}}$, only N process takes effect. Otherwise, when $\omega > \omega_{\text{limit}}$, there is U process only and the momentum direction should be re-sampled. So the relaxation times for the TA branch can be taken from Holland's work as

$$\frac{1}{\tau_{N,TA}} = B_T \omega T^4, \tag{72}$$

$$\frac{1}{\tau_{U,TA}} = \frac{B_{TU} \omega^2}{\sinh(\hbar\omega/k_B T)}. \tag{73}$$

For the LA branch, there is no frequency limit and only N process exists with the relaxation time

$$\frac{1}{\tau_{N,LA}} = B_L \omega^2 T^3. \quad (74)$$

Momentum conservation, or determining N- or U process while scattering happens, is difficult to address in MC method because each particle is dealt independently. As stated in previous chapter, U process contributes to thermal resistance while N process does not. Those can be prescribed as when the phonon scatter through U process, its direction would be randomly chosen just like the initial distribution so that it can be randomly scattered and contribute to the heat transport. On the other hand, the phonon through N process would not change its propagation direction.

In reality, the phonons destroyed by scattering are replaced almost at the same rate by a phonon of a near frequency. In the computation of relaxation time approximation [23], there is a frequency limit ω_{limit} corresponding to $q = q_{\text{max}}/2$ for the transverse branch. Below this limit there are no U processes, and above the limit, N process is no longer effective. On the other hand, longitudinal branch does not have frequency limit and only N process exists [7].

4.7 Re-Initialization

Modeling three-phonon scattering using MC method is quite challenging to address because MC tracks each particle while phonon system does not conserve the number of particles. Therefore, the number of the particles in the cell after scattering events should be adjusted by deleting or adding according to the cell energy. After each drift and scattering process, the phonons in each cell are randomly distributed and re-initialized. The distribution function is modified with the probability of scattering as

$$F_{\text{scat}}(\tilde{T}) = \frac{\sum_{j=1}^i N_j(\tilde{T}) \times P_{\text{scat},j}}{\sum_{j=1}^{N_b} N_j(\tilde{T}) \times P_{\text{scat},j}} \quad (75)$$

where $\tilde{T}$ means the actual temperature calculated after drift. If a phonon scatter in a U process, its direction after scattering is randomly chosen as in the initialization procedure. On the other hand, a phonon with an N process approximately preserve momentum, so it does not change its momentum direction Ω .

4.8 Results

The simulations on Si with various dimensions have been performed to show that the phonon MC can actually be a great way to calculate the thermal conductivity. When the temperature gradient is small enough and the simulation time is optimized, the thermal conductivity calculated by MC has been good match with the theoretical values. The simulation structures for Si at 300 K has following parameters:

- Temperature gradients: $T_h = 310\text{K}$ and $T_c = 290\text{K}$, (The temperature difference has been traditionally taken to be 20K.)
- Material structure: stack of 20 cells ($L_x = 50\text{nm}$, $L_y = 50\text{nm}$, $L_z = 200\text{nm} \times 20$),
- Time step $\Delta t = 1\text{ps}$,
- Number of super particles: 80,000

The simulation result for transient regime is shown in Figure 14. It is obvious that with longer simulation time (more than 30ns), the temperature gradient is linear without much noise.

The thermal conductivity is determined by the heat flux calculation. Simulations have been performed from 100K to 500K with $2\mu\text{m}$ thick slab. The total heat flux Φ is calculated along the z direction as

$$\Phi = \frac{1}{V} \sum_{n=1}^{N^*} W(\hbar\omega_n) \mathbf{v}_{gn} \cdot \mathbf{k}, \quad (76)$$

where W is weighting factor explained in Eq.(59). The thermal conductivity κ can be obtained in Fourier's regime when we take net flux $\phi = \Delta\Phi$ in cells as

$$\phi = \frac{1}{A\Delta t} \sum_{n=1}^{N^*} W(\hbar\omega_{n_in} - \hbar\omega_{n_out}) |\mathbf{q}_z| = \kappa \nabla T, \quad (77)$$

where A is cell area and Δt is the simulation time. The calculated value of the thermal conductivity at 300K is $\kappa_{Si} = 160 \text{ W m}^{-1} \text{ K}^{-1}$, and this value is in agreement to the analytical value from bulk data (fitted to experiments) as

Figure 14: Transient temperature in Fourier's regime for Si when $\Delta t=1\text{ps}$.

Figure 15: Silicon thermal conductivities; comparison between bulk (experimental) and MC simulation values.

$$\kappa_{\text{Si}} = \frac{\exp(12.570)}{T^{1.326}} = 149. \quad (78)$$

The Si value calculated from MC simulation result is quite comparable. Figure 15 shows the comparison between the bulk theoretical values and phonon MC simulation values. It gives good agreement above 200K. For lower temperatures below 200K, there is a gap between theory and simulation result. At low temperature, a phonon does not scatter frequently with other phonons, and the phonon mean free path is mainly limited by the boundary. Actually the experimental data from Ashegi's work on thin film show that the thermal conductivity at low temperature significantly decreases in comparison with bulk data [19]. That is due to reduction of phonon mean free path by boundaries.

For very low temperatures the phonons can propagate from hotter to colder end without colliding because the mean free path of the phonon becomes larger than the structure length. Figure 16 shows the transient temperature in the ballistic regime for Si in this case. For very low temperature,

$$T_{\text{ballistic}} = \left[\frac{T_h^4 + T_c^4}{2} \right]^{1/4} \quad (79)$$

The simulation result shows that when $T_h = 11.8$ K and $T_c = 3$ K, $T_{\text{ballistic}} = 10$ K after appropriate simulation time (25 ns).

Figure 16: Transient temperature in the ballistic regime for Si.

Chapter 5

Conclusion

The phonon MC simulation results show good agreement with the theoretical and experimental values for a range of temperatures. Thus, this will be a useful tool to simulate nano-scaled devices if the relaxation times are adjusted accordingly. Since MC method follows each phonon in every event, it is quite challenging to simulate realistic three phonon scattering. This study used the relaxation time values from Holland's work and simplified U- and N-process. However, Lacroix claims that direct calculation of phonon scattering relaxation time can be realized by using theoretical values of τ from Han and Klemens' work [23].

This work can be improved if the optical phonons are included. The optical phonons do not play significant role in terms of thermal conductivity, but contribute to modify the relaxation time through decaying into acoustic phonons. Also recent works indicate that it cannot be neglected for the capacitive properties [24].

For that matter, Molecular dynamics simulation is helpful to extract the parameters such as the relaxation times and the thermal conductivities. LAMMPS (Large scale Atomic/Molecular Massively Parallel Simulator) is the classical molecular dynamics simulator which models an ensemble of particles in a liquid, solid, and gaseous state. It consists of open source code of C++ and runs on single-processor desktop or parallel machine. LAMMPS is installed on Saguaro and has expanded resources on the website (<http://lammps.sandia.gov>). It actually has been proven successfully to be a good simulator for thermal conductivities of Si. Future work will be focused on combining phonon MC with device simulator using the parameters from LAMMPS simulator.

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