To my family
ACKNOWLEDGMENTS

First of all, I need to thank Prof. Jing Guo for his encouragement, guidance and patience. He taught me how to approach unexpected and complicated problems, which I encountered while working on this thesis, by always guiding me in the right direction. His concise explanations on device physics and computer programs have been of great help. I thank very much Professor Gijs Bosman and Ant Ural for serving on my committee, teaching device physics, and giving priceless advice on this work. I also thank my colleagues, Dr. Yijian Ouyang, Jason Seol, Yang Lu, Qun Gao, Wenchao Chen, Jyotsna Chauhan, Dr. Bala Kumar and Leitao Liu, for their collaboration.
# TABLE OF CONTENTS

ACKNOWLEDGMENTS.................................................................................................................. 4

LIST OF TABLES......................................................................................................................... 7

LIST OF FIGURES......................................................................................................................... 8

LIST OF ABBREVIATIONS............................................................................................................ 10

ABSTRACT .................................................................................................................................... 11

CHAPTER

1 INTRODUCTION ......................................................................................................................... 13

Contact ...................................................................................................................................... 13
Non-Equilibrium Green’s Function (NEGF)............................................................................... 14

2 SILICIDE SILICON CONTACT .................................................................................................. 18

N-type Silicon.............................................................................................................................. 18
   Physical Model ......................................................................................................................... 18
   Simulation Algorithm and Strategy .......................................................................................... 23
P-type Silicon.............................................................................................................................. 25
   Physical Model ......................................................................................................................... 25
   Simulation Algorithm and Strategy .......................................................................................... 27
Result ......................................................................................................................................... 27
   N-Type Silicon ......................................................................................................................... 27
   P-Type Silicon ......................................................................................................................... 28

3 SILICIDE GALLIUM ARSENIDE CONTACT ........................................................................... 44

Physical Model and Simulation Algorithm ............................................................................... 44
Result ......................................................................................................................................... 44
   N-type Gallium Arsenide.......................................................................................................... 44
   P-type Gallium Arsenide.......................................................................................................... 44

4 NUMERICAL INVESTIGATION ................................................................................................ 48

Simulation Environment ............................................................................................................ 48
Parallel Computing Performance Analysis ............................................................................... 48

5 NUMERICAL ISSUES .............................................................................................................. 53

Summation................................................................................................................................. 53
Integration................................................................................................................................. 54
<table>
<thead>
<tr>
<th>Poisson Equation</th>
<th>55</th>
</tr>
</thead>
<tbody>
<tr>
<td>6  CONCLUSION</td>
<td>59</td>
</tr>
</tbody>
</table>

**APPENDIX**

<table>
<thead>
<tr>
<th>THE FORTRAN CODE FOR THE ADAPTIVE SIMPSON ALGORITHM</th>
<th>60</th>
</tr>
</thead>
<tbody>
<tr>
<td>LIST OF REFERENCES</td>
<td>63</td>
</tr>
<tr>
<td>BIOGRAPHICAL SKETCH</td>
<td>65</td>
</tr>
</tbody>
</table>
## LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-1</td>
<td>52</td>
</tr>
<tr>
<td>Runtime (16 CPUs) for all simulation programs</td>
<td>52</td>
</tr>
<tr>
<td>Figure</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>1-1</td>
<td>Band profile of silicide n-type silicon contact</td>
</tr>
<tr>
<td>1-2</td>
<td>Device structure of a channel with source and drain</td>
</tr>
<tr>
<td>2-1</td>
<td>The effective mass model and silicide silicon (n-type) contact</td>
</tr>
<tr>
<td>2-2</td>
<td>Image charge</td>
</tr>
<tr>
<td>2-3</td>
<td>Image potential energy</td>
</tr>
<tr>
<td>2-4</td>
<td>Flow chart of parallel algorithm for n-type silicon</td>
</tr>
<tr>
<td>2-5</td>
<td>The band diagram of the silicide silicon (p-type) contact</td>
</tr>
<tr>
<td>2-6</td>
<td>Conduction band profile for Nd=1.9e20.</td>
</tr>
<tr>
<td>2-7</td>
<td>Conduction band profile for Nd=3.3e18</td>
</tr>
<tr>
<td>2-8</td>
<td>Transmission for n-type silicon</td>
</tr>
<tr>
<td>2-9</td>
<td>Comparison between the transmission and the conduction band</td>
</tr>
<tr>
<td>2-10</td>
<td>The multiplication of the transmission and the thermal broadening function for n-type Si</td>
</tr>
<tr>
<td>2-11</td>
<td>The resistances calculated from (2-2, solid line) and (2-7, diamond line)</td>
</tr>
<tr>
<td>2-12</td>
<td>The simulation and experimental data for silicide n-type silicon contact</td>
</tr>
<tr>
<td>2-13</td>
<td>The resistances over various barrier heights</td>
</tr>
<tr>
<td>2-14</td>
<td>Valence band profile for Na=3e20.</td>
</tr>
<tr>
<td>2-15</td>
<td>Valence band profile for Na=1.7e18.</td>
</tr>
<tr>
<td>2-16</td>
<td>Transmission for p-type silicon</td>
</tr>
<tr>
<td>2-17</td>
<td>The multiplication of the transmission and the thermal broadening function for p-type silicon</td>
</tr>
<tr>
<td>2-18</td>
<td>Comparison between the transmission and the valence band.</td>
</tr>
<tr>
<td>2-19</td>
<td>The simulation and experimental data for silicide p-type silicon contact</td>
</tr>
<tr>
<td>3-1</td>
<td>The resistances from numerical integration and 2D Fermi function</td>
</tr>
</tbody>
</table>
Comparison between n-type GaAs and n-type Si simulation resistances .......... 46
p-type GaAs and p-type Si simulation resistances. ........................................ 47
Parallel algorithm runtime ........................................................................ 50
Parallel algorithm speedup ........................................................................ 51
Parallel algorithm efficiency ...................................................................... 52
P(E,a,b) plot .............................................................................................. 57
Three examples of inappropriate tolerance for the Simpson algorithm ........ 58
Tunning integral value for the Simpson algorithm ...................................... 58
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>NEGF</td>
<td>Non-equilibrium Green's function</td>
</tr>
<tr>
<td>MOSFET</td>
<td>Metal-oxide-semiconductor field-effect transistor</td>
</tr>
<tr>
<td>GHz</td>
<td>Giga Hertz</td>
</tr>
<tr>
<td>GB</td>
<td>Giga Bityes</td>
</tr>
<tr>
<td>CPU</td>
<td>Central processing unit</td>
</tr>
<tr>
<td>ID</td>
<td>Identification</td>
</tr>
<tr>
<td>2D</td>
<td>Two dimensions</td>
</tr>
</tbody>
</table>
Abstract of Thesis Presented to the Graduate School of the University of Florida in Partial Fulfillment of the Requirements for the Degree of Master of Science

PARALLEL SIMULATION OF NICKEL SILICIDE SILICON AND NICKEL SILICIDE GALLIUM ARSENIDE CONTACT RESISTANCE IN A WIDE DOPING RANGE

By

Dukjin Kim

August 2011

Chair: Jing Guo
Major: Electrical and Computer Engineering

Scaling of solid-state devices has been successful during the past 40 years. As device feature size reduced, the density of transistors in a single chip has increased and this improved cost and performance. However, no one is sure if Moore’s law would continue for the next decade due to the barriers to extend scaling such as gate tunneling, subthreshold channel leakage, device parameter variability, parasitic resistance and capacitance.

There have been intensive efforts to continue Moore’s law. Current research efforts are mainly focused on new channel material to improve carrier mobility. However, it is reported that parasitic effect including contact resistance is also a serious limiting factor.

In this thesis, simulation of specific resistances of NiSi/Si contact and NiSi/GaAs contact in a broad doping range for n-type and p-type dopants are presented. The simulated Si resistances are compared to experimental data, but the simulated GaAs resistances are compared to the simulated Si resistances due to lack of experimental data. Simulation has been performed by parallel computing and the non-equilibrium Green’s function (NEGF) formalism is used for modeling the ballistic transport in the
contact. For parallel programming, FORTRAN with the Message Passing Interface (MPI) is used.
CHAPTER 1
INTRODUCTION

Contact

One of the main purposes of scaling solid-state device is to improve the density of transistors and the circuit speed. Increasing density is crucial to reduce manufacturing cost and fast circuit speed is needed to improve the device performance. Scaling device size guarantees higher transistor density. Nonetheless, device speed cannot be increased proportionally with physical device size. The metal-oxide-semiconductor field-effect transistor (MOSFET) structure has an intrinsic parasitic resistance which cannot be scaled down proportionally with feature size and as a result, it degrades speed significantly [1], [2]. The intrinsic parasitic resistance includes contact resistance and diffusion sheet resistance. Both of the resistances are important with respect to speed degradation. However, the contact resistance is considered to be the most serious component [3], [4].

The silicide-diffusion contact has been employed to reduce the contact resistance. The silicide-diffusion contact is a Schottky contact. The band profile for silicide n-type Si contact is shown in Fig. 1-1. The contact in this thesis is phenomenologically modeled. The energy level of the bottom of the Fermi sea of silicide is set to be low enough to mimic the real contact. This value is -2eV for n-type material and 2eV for p-type material. The barrier height is fitted using the experimental data [5]. If we assume that a Schottky contact is formed at one end of the semiconductor, the band profile at the other end is assumed to be flat to make the transmission perfect. The Fermi level is set to be at zero.
Non-Equilibrium Green’s Function (NEGF)

The NEGF formalism is widely used for nanoscale device modeling [6], [7]. In the NEGF formalism, the device shown in Fig. 1-2 is described by a Hamiltonian (H), self-energies ($\Sigma_1$, $\Sigma_2$) and overlap matrix (S) for the ballistic transport. The Hamiltonian includes band structure information. Eigen values of the Hamiltonian are energy states of the channel. The self-energies represent coupling between the source and the channel and between the drain and the channel. Specifically, discrete energy levels of the channel are broadened and become continuous due to the formation of contact. This phenomenon is described by self-energy terms. The overlap matrix presents the excitation effect of the channel due to electron waves leaking into the channel from the contact. For incoherent transport case, additional term, $\Sigma_{\text{Scat}}$, is needed to capture the scattering mechanism. In this thesis, only ballistic transport is considered.

Now, we can write the retarded Green’s function, G, for the channel at energy $E$

$$G = [(E + i0^+)S - H - U - \Sigma_1 - \Sigma_2]^{-1}$$  \hspace{1cm} (1-1)

where $0^+$ is a positive infinitesimal and $U$ is self-consistent potential in the channel calculated by the Poisson solver. Under equilibrium case, the density of states (DOS) is defined as

$$DOS = \frac{1}{2\pi} \text{Trace}[A(E)]$$  \hspace{1cm} (1-2)

where the spectral function, $A(E)$, is calculated from G.

$$A(E) = i[G - G^+]$$  \hspace{1cm} (1-3)

The density matrix, $[\rho_e]$, is

$$[\rho_e] = \int_{-\infty}^{\infty} \frac{dE}{2\pi} f(E - \mu)[A(E)]$$  \hspace{1cm} (1-4)
where $\mu$ is the equilibrium Fermi level and $f(E-\mu)$ is the Fermi-Dirac distribution function.

$$f(E-\mu) = \frac{1}{1 + \exp\left(\frac{E-\mu}{k_B T}\right)}$$

(1-5)

where $k_B$ is the Boltzmann constant and $T$ is the temperature.

Under non-equilibrium condition, we have two different spectral functions ($A_1, A_2$) and Fermi functions ($f_1, f_2$) for the source and drain, respectively. The density matrix is now defined as

$$[\rho_c] = \int_{-\infty}^{\infty} \frac{dE}{2\pi} \left( f(E-\mu_1)[A_1(E)] + f(E-\mu_2)[A_2(E)] \right)$$

(1-6)

where

$$A_1 = G \Gamma_1 G^+$$

(1-7)

$$A_2 = G \Gamma_2 G^+$$

(1-8)

$$\Gamma_{1,2} = i[\Sigma_{1,2} - \Sigma_{1,2}^+]$$

(1-9)

$\Gamma_{1,2}$ is called the Broadening matrix and represents the energy level broadening effect.

The density matrix equation, (1-6), implies that, if $\mu_1 > \mu_2$, the source pumps electrons into the channel until the channel Fermi level is equal to $\mu_1$, and the drain takes electrons out of the channel until the channel Fermi level is equal to $\mu_2$. However, neither the source nor the drain can be in equilibrium with the channel. This process takes place continuously as long as $\mu_1 > \mu_2$. This mechanism explains how electron density in the channel is determined and how electrons flow through the device.

Coherent transport is usually described by transmission formalism. Transmission, $T(E)$, is calculated as follows.

$$T(E) = \text{trace}[\Gamma_1 A_2] = \text{trace}[\Gamma_2 A_1]$$

(1-10)
With $T(E)$ and the Fermi functions for the source and drain, the current is defined as

$$I = \frac{q}{\hbar} \int_{-\infty}^{\infty} dET(E)(f(E - \mu_1) - f(E - \mu_2))$$

(1-11)

This is a one dimensional current. Spin degeneracy is not taken into consideration here. The derivative of the Fermi function in the current equation (1-11) gives conductance, $C$.

$$C = \frac{q^2}{\hbar} \int_{-\infty}^{\infty} dET(E)F_T(E - \mu)$$

(1-12)

where the thermal broadening function, $F_T(E)$, is defined as

$$F_T(E) = -\frac{\partial f(E)}{\partial E}$$

(1-13)

The resistance, $\rho$, is calculated from $C$.

$$\rho = \frac{1}{C} \quad [\Omega]$$

(1-14)
Figure 1-1. Band profile of silicide n-type Si contact.

Figure 1-2. Device structure of a channel with source and drain. $\mu_1$ and $\mu_2$ are the Fermi levels of the source and the drain, respectively. Hamiltonian matrix, $H$, contains the band structure information of the channel. Self-energies, $\Sigma_1$ and $\Sigma_2$, represent the coupling between the source and the channel and between the drain and the channel, respectively. The overlap matrix, $S$, describes the excitation of the channel due to the formation of the contact.
CHAPTER 2
SILICIDE SILICON CONTACT

N-type Silicon

Physical Model

For n-type Silicon, one band effective mass model discretized by the finite difference method is employed (see Fig. 2-1 top). The model is valid due to the fact that energy levels in the conduction band are parabolic, isotropic and well separated from each other. The silicide silicon contact is basically a Schottky contact. This contact is phenomenologically modeled (see Fig. 2-1 bottom). The silicide Fermi energy level, $E_m$, which is equal to the conduction band edge of silicide and the silicon Fermi energy level, $E_F$, are set to be at zero. Open boundary condition is applied at the side of the silicon which is opposite to the Schottky contact. The barrier height, $\Phi_{bn}$, is fitted using the experimental data [5]. The energy level of the bottom of the Fermi sea is assumed to be -2eV. The image charge barrier lowering is also considered.

In the previous chapter, conductance equation is derived as,

$$C = \frac{q^2}{h} \int_{-\infty}^{\infty} dET(E)F_T(E - \mu) \tag{1-12}$$

This is a one dimensional equation and a two dimensional cross-section area is not taken into consideration. Let us assume that transport is in z-direction and the cross-sectional area is in (x, y) space. To cover (x, y) space, we simply do a summation of (1-12) over a $(k_x, k_y)$ space with assumption that periodic boundary conditions are applied and the transverse modes are not coupled. There are two methods of this summation,

$$\frac{C}{S} = \frac{q^2}{S \cdot h} \sum_{k_x, k_y} \int_{-\infty}^{\infty} dET(E + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_e})F_T(E - \mu) \tag{2-1}$$
and

$$\frac{C}{S} = \frac{q^2}{S \cdot h} \sum_{k_x, k_y} \int_{-\infty}^{\infty} dE T(E) F_r(E - \mu + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_c})$$

(2-2)

where $m_c$ is conduction band effective mass. Transmission, $T(E)$, is dependent on $k_x$, $k_y$ and $k_z$. Therefore, (2-1) is correct. But, because $(k_x, k_y)$ modes are all decoupled, transmission is just shifted by the $(k_x, k_y)$ modes. Moreover, we do the summation over the entire $(k_x, k_y)$ space. This proves that (2-2) gives the same result as (2-1). The unit of conductance from the two equations is [simens/m²]

There is another way to take the cross-sectional area into consideration for conductance. The following is the current equation derived in the previous chapter.

$$I = \frac{q}{h} \int_{-\infty}^{\infty} dE T(E) (f(E - \mu_1) - f(E - \mu_2))$$

(1-11)

This is a one dimensional current equation. We can do summation of this equation over $(k_x, k_y)$ space.

$$\frac{I}{S} = \frac{q}{S \cdot h} \sum_{k_x, k_y} \int_{-\infty}^{\infty} dE T(E + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_c}) (f(E - \mu_1) - f(E - \mu_2))$$

(2-3)

$$\frac{I}{S} = \frac{q}{S \cdot h} \sum_{k_x, k_y} \int_{-\infty}^{\infty} dE T(E) \left( f(E - \mu_1 + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_c}) - f(E - \mu_2 + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_c}) \right)$$

(2-4)

(2-3) and (2-4) are equivalent for the same reason as in the (2-1) and (2-2) case. We can change (2-4) into an analytical expression by introducing a two dimensional Fermi function, $f_{2D}(E)$, [8].

$$\frac{1}{S} \sum_{k_x, k_y} f \left( E + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_c} \right)$$
\[
\int_0^{2\pi k_T} \frac{1}{4\pi^2} \frac{1}{1 + A \exp(\hbar^2 k^2 / (2m k_B T))} \, dk
\]

where \( A = \exp(E / k_B T) \)

\[
= \frac{m k_B T}{2\pi h^2} \int_0^\infty \frac{dy}{1 + Ae^y}
\]

\[
= \frac{m k_B T}{2\pi h^2} \ln \left[ A e^{-y} \right]_0^\infty
\]

\[
= \frac{m k_B T}{2\pi h^2} \ln[1 + \exp(-E / k_B T)] = f_{2D}(E)
\] (2-5)

Replacing \( f(E) \) by \( f_{2D}(E) \) in (2-4),

\[
\frac{I}{S} = \frac{q}{\hbar} \int_\infty^\infty \! dE T(E) (f_{2D}(E - \mu_1) - f_{2D}(E - \mu_2))
\] (2-6)

Conductance is the derivative of (2-6).

\[
\frac{C}{S} = \frac{q^2}{\hbar} \int_\infty^\infty \! dE T(E) \left( \frac{\partial f_{2D}(E)}{\partial E} \right)_{E=E_0}
\] (2-7)

Transmission is needed to calculate conductance. As shown in chapter 1, we can find transmission using overlap matrix, Hamiltonian, self-energy and potential profile.

First, overlap matrix is an identity matrix. This is because only orthonormal basis functions are used in this one band effective mass model. Hamiltonian matrix is shown as

\[
H = \begin{bmatrix}
(E_1 + 2t_1) & -t_1 \\
-t_1 & (E_2 + t_1 + t_2) & -t_2 \\
-t_2 & (E_3 + 2t_2) & -t_2 \\
& & & \ddots & \ddots \\
& & & & \ddots & \ddots \\
& & & & & \ddots & \ddots \\
& & & & & & \ddots & \ddots & -t_2 (E_N + 2t_2)
\end{bmatrix}
\] (2-8)
\( t_1: \) silicide bonding energy

\( t_2: \) silicon bonding energy

\( E_c - E_N: \) conduction band profile

H is a sparse matrix because only three diagonal elements are non-zero. If N atoms are used for modeling, size of H is N \times N. In Fig. 2-1 top, the leftmost atom represents a silicide atom. The next atom is in the intersection between silicide and silicon. The rest of the atoms are silicon. Likewise, H(1,1) is a silicide atom, H(2,2) is an atom in the intersection and H(3,3) \sim H(N,N) are silicon atoms. Self-energy is an N \times N sparse matrix, too. It has only one non-zero element.

\[
\Sigma_1(1,1) = -t_2 \exp(ik_1) \tag{2-9}
\]

\[
\Sigma_2(N,N) = -t_2 \exp(ik_2) \tag{2-10}
\]

where \( k_1 \) and \( k_2 \) are wavenumbers and can be calculated from the dispersion relation.

\[
h(k) = E_c + 2t_0(1 - \cos(ka)) \tag{2-11}
\]

\( k: \) wavenumber

\( E_c: \) conduction band profile

\( t_0: \) bonding energy

\( a: \) atomic distance

Potential, U, is calculated self-consistently from the Poisson equation and the Boltzmann-Maxwell approximation equation.

\[
n(z) = N_c \exp\left(-\frac{(E_c(z) - E_F)}{k_BT}\right) \tag{2-12}
\]

\[
-\frac{d}{dz}\left(\varepsilon_r \frac{dU}{dz}\right) = \frac{q^2}{\varepsilon_0} n(z) \tag{2-13}
\]
\( n(z) \): electron density at \( z \)

\( \varepsilon_r \): relative permittivity

\( \varepsilon_0 \): permittivity of free space

\( N_c \): effective density of states at conduction band

First, a guessed initial value of \( U \) is used to calculate \( n(z) \) value from (2-12). \( E_c \) is equal to \(-q \times U\). Next, \( U \) is calculated from (2-13) using the \( n(z) \) value. This \( U \) value is compared to the initial \( U \) value. If the difference is too large, the process is repeated again. This process is repeated until the error is within an allowed error range. The image charge effect should be included in the potential energy profile. Let us assume that there is negative charge (-q) inside silicon and the distance between the negative charge and the surface of metal is \( x \) (Fig 2-2). An equal amount of positive charge will be induced at the surface due to the negative charge. The induced surface charge can be replaced by positive charge (+q) at a distance \(-x\) from the metal surface. This charge is called the image charge. There is an attractive force between the negative charge and image charge.

\[
F = \frac{-q^2}{16\pi\varepsilon_0 x^2}
\]  

(2-14)

\( F \) is called the image force. The amount of work to bring an electron from infinity to the point \( x \) is

\[
E(x) = \int_x^\infty Fdx = \frac{q^2}{16\pi\varepsilon_0 x}
\]  

(2-15)

By definition, \( E(x) \) is electron potential energy at a distance \( x \) from the metal surface and is shown in Fig. 2-3. As a consequence, the Schottcky barrier is lowered by \( E(x) \) and
this phenomenon is referred to as the image charged induced barrier lowering. E(x) should be added to E_c and next, E_c is added to the diagonal elements of Hamiltonian as shown in (2-8).

**Simulation Algorithm and Strategy**

The three expressions for conductance are,

\[ \frac{C}{S} = \frac{q^2}{S \cdot h} \sum_{k_x, k_y} \int_{-\infty}^{\infty} dE T(E) \left( E + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_c} \right) F_T(E - \mu) \]  

(2-1)

\[ \frac{C}{S} = \frac{q^2}{S \cdot h} \sum_{k_x, k_y} \int_{-\infty}^{\infty} dE T(E) F_T(E - \mu + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_c}) \]  

(2-2)

\[ \frac{C}{S} = \frac{q^2}{h} \int_{-\infty}^{\infty} dE T(E) \left( - \frac{\partial f_{2D}(E)}{\partial E} \right)_{E=\mu} \]  

(2-7)

(2-7) requires the least amount of computation because it is an analytical equation. (2-1) computes T(E) as many times as the number of grid points in (k_x, k_y) summation space and (2-2) computes F_T(E) over the same number of gird points. Less computational effort is required in computing F_T(E), hence, (2-2) is more efficient then (2-1). In this thesis, (2-2) and (2-7) are adapted to simulate conductance. The results from the two algorithms will be compared. (2-7) contains no parallel workload and therefore its algorithm should be performed by serial program. On the other hand, (2-2) has good parallel workload i.e. summation.

The parallel algorithm flow chart is given in Fig. 2-4. One processor is named master and other processors are named slaves. First, the master processor calculates the self-consistent potential energy which is the conduction band edge, E_c. The following step is the summation of the thermal broadening function over (k_x, k_y) space. This step requires the largest computation workload and is parallelized. Let us assume...
that grid points for \( k_x \) are in a range from 1 to \( r \). For simplicity, \( k_y \) grid points are assumed to be from 1 to \( r \), as well. Summation over a two dimensional space could be performed by two loops: one for \( k_x \) and another for \( k_y \). Parallelization could be achieved by dividing one of the two loops. All of the processors perform summation over the entire \( k_y \) grid but only a part of \( k_x \) grid. If the number of the processors is \( p \), \( r/p \) of \( k_x \) grid points is assigned to each of the processors. The range, 1 to \( r \), should be appropriately assigned. Each processor should be aware of which part of the range it should work on. This is done using processor IDs. Each of the processors has its own ID from 0 to \( (p-1) \). Once \( r \) is decided, the specific range for each of the processors is decided through the IDs. To initiate the slave processors, the master broadcasts parameters for summation of the thermal broadening function and finalizing flag \( (=0) \) to the slave processors using MPI_BCAST. MPI_BCAST is a collective communication function and is more efficient than a one-to-one communication function where one processor sends the same data to all processors. While the slaves are working on the summation, the master also performs the summation in the assigned range. Next, the master collects the summed data from the slaves using MPI_GATHER. MPI_GATHER is also a collective communication function and is efficient when one processor receives data from all other processors. The master sums the collected data. The resulting value is named \( f_{\text{prime}} \). Next, transmission is calculated. \( f_{\text{prime}} \) weighted by transmission is input (integrand) to the integration algorithm which uses the adaptive Simpson rule. This algorithm is recursively repeated until the integral value is within predefined error. If the algorithm needs to be repeated with another input when the integral value is out of the error, the master goes back to the broadcasting step. Otherwise, the master finalizes the slaves
by broadcasting finalizing flag (=1). The resistance value is printed and the master terminates.

**P-type Silicon**

**Physical Model**

The energy levels in valence band are spaced closely and they are significantly anisotropic and non-parabolic. One band effective mass model is not valid for the valence band. Instead, three bands effective mass model is adapted. The heavy hole, light hole and spin-orbit split-off bands are used. In the case of n-type silicon, the one dimensional transmission is just shifted by additional \((k_x, k_y)\) modes and the shape of transmission plot remains unchanged. It could be easily understood because all the modes are assumed to be decoupled. This assumption is no longer valid for the valence band case. Transmission with additional \((k_x, k_y)\) mode is shifted from the original transmission and its shape also changes. Therefore, mathematical techniques for (2-2) and (2-7) cannot be applied here. Instead, conductance equation is given as follows,

\[
\frac{C}{S} = \frac{q^2}{S \cdot h} \sum_{k_x, k_y} \int_{-\infty}^{\infty} dE T(E, k_x, k_y) F_y(E - \mu)
\]

\[(2-8)\]

The dispersion relation is shown in (2-9) [9]. The Luttinger parameters are material dependent [10]. (2-9) is discretized by the finite difference method and the resulting matrix is a Hamiltonian matrix. If \(N\) atoms are used in this model, the Hamiltonian is a \(6N \times 6N\) block tridiagonal matrix. \(\Sigma_1\) is \(6N \times 6N\) sparse matrix and only the first \(6 \times 6\) block contains non-zero elements. \(\Sigma_2\) has non-zero values in the last \(6 \times 6\) block. The self-energies are calculated by the Sancho-Rubio approach [11]. Overlap matrix is an identity matrix and the potential energy is calculated through the same procedure as for the n-type case.
The band diagram for p-type contact is depicted in Fig. 2-5. As in n-type contact, the contact at the side opposite to the Schottky contact of silicon is treated by open boundary condition. $E_F$ and $E_m$ are set to be at zero and the Schottky barrier is fitted to experimental data. The energy level of the bottom of the Fermi Sea for silicide is assumed to be 2eV.

\[
\begin{bmatrix}
P + Q & -S & R & 0 & -\frac{1}{\sqrt{2}}S & \sqrt{2}R \\
-S^+ & P - Q & 0 & R & -\sqrt{2}Q & \frac{3}{\sqrt{2}}S \\
R^+ & 0 & P - Q & S & \sqrt{3}S + & \sqrt{2}Q \\
0 & R^+ & S^+ & P + Q & -\sqrt{2}R & -\frac{1}{\sqrt{2}}S^+ \\
-\frac{1}{\sqrt{2}}S^+ & -\sqrt{2}Q & \frac{3}{\sqrt{2}}S & -\sqrt{2}R & P + \Delta & 0 \\
\sqrt{2}R^+ & \frac{3}{\sqrt{2}}S^+ & \sqrt{2}Q & -\frac{1}{\sqrt{2}}S & 0 & P + \Delta
\end{bmatrix}
\]

where

\[
P = \left(\frac{\hbar^2}{2m_0}\right)\gamma_1 \left(k_x^2 + k_y^2 + k_z^2\right)
\]

\[
Q = \left(\frac{\hbar^2}{2m_0}\right)\gamma_2 \left(k_x^2 + k_y^2 - 2k_z^2\right)
\]

\[
R = \left(\frac{\hbar^2}{2m_0}\right)\sqrt{3} \left[ -\gamma_2 \left(k_x^2 - k_y^2\right) + 2i\gamma_3 k_x k_y \right]
\]

\[
S = \left(\frac{\hbar^2}{2m_0}\right)2\sqrt{3}\gamma_3 \left(k_x - ik_y\right)k_z
\]

26
\gamma_1, \gamma_2, \gamma_3: \text{The Luttinger parameters}

\Delta: \text{The spin–orbit split–off energy}

**Simulation Algorithm and Strategy**

The main frame of the p-type algorithm is the same as that of the n-type algorithm. Only the summation part of (2-8) is parallelized.

\[
\sum_{k_x, k_y} T(E, k_x, k_y)
\]  

(2-10)

The difference is that \(T(E, k_x, k_y)\) is summed rather than \(F_T(E, k_x, k_y)\). The summation of \(T(E, k_x, k_y)\) needs the self-consistent potential energy. The potential energy could be calculated by master processor and broadcasted to the slave processors. However, when \(N\) atoms are used for the effective mass modeling, double precision buffer, which has a size of \(N\), is needed for the broadcasting. Communication time is the main source of overhead in parallel computing. Furthermore, calculating potential energy algorithm is quite fast. Therefore, it is time saving that every processor calculates the potential energy and saves it in its own memory.

**Result**

**N-Type Silicon**

The contact resistance is simulated over ten doping concentrations (Nd) in a range from 3.3e18 to 1.9e20. The conduction band profiles of the highest and lowest doping case are given in Fig. 2-6 and Fig. 2-7. Fig. 2-6 has thinner barrier width as expected. For Nd=1.9e20, the lowest conduction band edge is at about -0.1eV and accordingly transmission should start to increase from zero around this energy. This is shown in Fig. 2-8. The transmission does not reach its maximum value even at 5eV. This is due to the quantum reflection effect. The maximum value is six because there are six valleys at the
Si conduction band edge. In Fig. 2-9, the transmission is compared to the conduction band over an identical energy range. The conductance is obtained from the multiplication of transmission and the thermal broadening function. The resulting function is depicted in Fig. 2-10. The resistances from (2-2) and (2-7) are shown in Fig. 2-11. The two values are well matched proving that the numerical integration is accurate. In Fig. 2-12, the simulation and experimental data are plotted. The barrier height is fitted using the experimental value for the lowest doping concentration case. The lowest concentration experimental value is chosen because in low doping concentration the effect of the barrier height on the resistance is more significant. Fig. 2-13 shows the resistances simulated over the five different barrier heights. The resistance varies with the barrier height more significantly in low concentration.

**P-Type Silicon**

The p-type doping (Na) is in a range from 1.7e18 to 3e20 for the resistance simulation. The valence band profiles are given in Fig. 2-14 and Fig. 2-15 for the highest and lowest doping cases, respectively. The transmission which is flipped compared to n-type case is shown in Fig. 2-16. The maximum transmission is also six because three bands including the heavy hole, light hole and spin-orbit split-off bands are used and spin degeneracy is included. The resulting function from the multiplication of the transmission and thermal broadening function has the same shape with n-type case, as shown in Fig. 2-17. The valence band profile is compared to the transmission over an identical energy range in Fig. 2-18. The simulated resistance and experimental data are given in Fig. 2-19. The barrier height is tuned using the ninth point.
Figure 2-1. The effective mass model and silicide silicon (n-type) contact. A) $t_1$ and $t_2$ are bonding energies and $a$ is atomic distance. B) The contact is phenomenologically modeled. The Fermi level ($E_m$ for silicide, $E_F$ for silicon) is set to be at zero and the barrier height, $\Phi_{bn}=0.499\text{eV}$ is fitted using the experimental data. The energy level of the bottom of the Fermi sea for silicide is set to be at $-2\text{eV}$. 
Figure 2-2. Negative charge inside the silicon induces positive surface charge on the metal. This surface charge can be replaced by equal positive charge located inside the metal. The distance of the positive charge and negative charge from the metal surface is equal.

Figure 2-3. The dotted line indicates the image potential energy profile created by the positive image charge inside the metal. The image potential energy is added to the self-consistent potential energy calculated by the Poisson solver and it lowers the Schottky barrier.
Figure 2-4. Flow chart of parallel algorithm for n-type silicon. Only the summation part is parallelized.
Figure 2-5. The band diagram of the silicide silicon (p-type) contact. The Fermi level (Em for silicide, EF for silicon) is set to be at zero and the barrier height, \( \Phi_{bp} = 0.44\text{eV} \) is fitted using the experimental data. The energy level of the bottom of the Fermi sea for silicide is set to be at 2eV.

Figure 2-6. Conduction band profile for Nd=1.9e20.
Figure 2-7. Conduction band profile for Nd=3.3e18.
Figure 2-8. Transmission is zero below -0.1eV due to the bandgap and it starts to rise around -0.1eV. The transmission does not reach its maximum value immediately because of quantum reflection.

Figure 2-9. Comparison between the transmission and the conduction band. A) Transmission. B) Conduction band profile. Y-axis is energy for A) and B).
Figure 2-10. The multiplication of the transmission and the thermal broadening function for n-type Si.
Figure 2-11. The resistances calculated from (2-2, solid line) and (2-7, diamond line) are compared. The two values are well matched proving that the numerical integration in (2-7) is accurate.
NiSi/n-Si ($\Phi_{bn} = 0.499eV$)

Simulation Data
Experimental Data

Figure 2-12. The simulation and experimental data are plotted. The barrier height fitted using the experimental value of the highest concentration is 0.499eV.
Figure 2-13. The resistances over various barrier heights. The effect of barrier height is more prominent in low concentration.
Figure 2-14. Valence band profile for Na=3e20.
Figure 2-15. Valence band profile for Na=1.7e18.
Figure 2-16. Transmission for p-type Si. The transmission starts to increase from zero at around 0.2eV which is the top of the valence band. It does not reach its maximum value even below the contact barrier due to the quantum reflection.
Figure 2-17. The multiplication of the transmission and the thermal broadening function for p-type Si.

Figure 2-18. Comparison between the transmission and the valence band. A) Transmission. B) Valence band. Y-axis is energy for A) and B).
Figure 2-19. The simulation and experimental data. The barrier height fitted using the experimental value of the second highest concentration is 0.44eV.
CHAPTER 3
SILICIDE GALLIUM ARSENIDE CONTACT

Physical Model and Simulation Algorithm

Physical model and simulation algorithm for n-type and p-type Gallium Arsenide are corresponding to that of Silicon except material property constants such as the effective mass for n-type and the Luttinger parameter for p-type.

Result

N-type Gallium Arsenide

The simulation data from the 2D Fermi function and numerical integration are well matched as shown in Fig. 3-1. Because the experimental data does not exist, GaAs resistance is compared to Si resistance in Fig. 3-2. The same barrier height and doping concentrations are used for GaAs and Si. GaAs resistance is expected to be lower due to the lighter effective mass over all doping concentrations. However, GaAs has higher resistance for the first two points in Fig. 3-2. This can be explained as follows. In low doping case, the dominant transport mechanism is thermionic emission. Therefore, GaAs which has lighter effective mass shows lower resistance. On the other hand, in high doping case, tunneling mechanism is dominant. Si has six modes coming from the six valleys and GaAs has only one mode. When all modes have high transmission due to the thin barrier width, Si could have lower resistance.

P-type Gallium Arsenide

P-type GaAs resistance is also compared with Si resistance in Fig. 3-3 due to lack of experimental data. The barrier height and doping concentrations are fixed for the two materials. GaAs has always lower resistance and this is consistent with the fact that GaAs has lighter effective mass, and GaAs and Si have the same number of modes.
n-GaAs ($\Phi_{bn}=0.499$eV)

$1/sqrt(N_d)$ ($10^{-10}$ cm$^{3/2}$)

Numerical Integration

2D Fermi Function

Figure 3-1. The resistances from numerical integration and 2D Fermi function are well matched proving that the numerical integration is accurate.
Figure 3-2. n-type GaAs and n-type Si simulation resistances are compared. The barrier height and doping concentrations are fixed for the two materials. In low concentration, GaAs resistance is lower because the effective mass in GaAs is lighter. In high concentration, Si resistance is lower because Si has six transmission modes and GaAs has only one transmission mode.
Figure 3-3. p-type GaAs and p-type Si simulation resistances are plotted. GaAs has always lower resistance. This is because the number of transmission modes of p-type GaAs is equal to that of p-type Si, and p-type GaAs has a lighter effective mass.
CHAPTER 4
NUMERICAL INVESTIGATION

Simulation Environment

The simulation programs have been written in FORTRAN with the Math Kernel Library (MKL). For parallel computing, the Message Passing Interface (MPI) is used. The programs are run on the University of Florida High Performance Computing (HPC) Center where each computing nodes has 4 to 8 cores (2.2 to 2.8 GHz) and 4 to 64 GB memory (2.7 GB per one core on average). There are a total of 3854 cores in the HPC center.

Parallel Computing Performance Analysis

In parallel computing, processors interact with each other by sending and receiving data. The time needed for the data to be transferred from one processor to another processor(s) is defined as communication time. The total parallel runtime consists of computation time and communication time. The communication time is the main source of overhead which is defined below,

\[ T_o = pT_p - T_s \]  

(4-1)

where

- \( T_o \): overhead
- \( p \): number of processors
- \( T_p \): parallel runtime
- \( T_s \): serial runtime

\( T_p \) is the time taken from the start of parallel program to the moment when the last processing unit finishes working. \( T_s \) is the runtime when the program is run on a single processor. There are three main performance metrics for parallel systems: runtime, speedup and efficiency [12]. N-type Si simulation algorithm is analyzed by the metrics. Fig. 4-1 shows the runtime. The runtime continuously decreases until 16 CPUs, but
after that, the runtime actually increases. This is due to the fact that as more processing units are used, the communication time becomes more significant. Once the communication time is comparable to computation time, we cannot obtain any benefit from parallelization. Speedup is

\[
S = \frac{T_s}{T_p}
\]  \hspace{1cm} (4-2)

and is shown in Fig.4-2. S reaches the peak value at 16 CPUs. Therefore, the optimal number of processing units for this algorithm is 16. Efficiency is always less than or equal to 1 due to the overhead and drops as more CPUs are used (see Fig. 4-3). In Table 4-1, runtimes for all simulation algorithms are given.
Figure 4-1. Runtime decreases until 16 CPUs and after that it increases. Beyond 16 CPUs, the overhead (communication time) is dominant and we cannot obtain any benefit from parallelization.
Figure 4-2. Speedup increases until 16 CPUs and drops after that. The optimal number of CPUs for this parallel algorithm is 16.
Figure 4-3. Efficiency is always less than or equal to 1 due to the overhead. Continuously dropping E implies that the overhead continuously increases.

<table>
<thead>
<tr>
<th>Material</th>
<th>n-type Si</th>
<th>p-type Si</th>
<th>n-type GaAs</th>
<th>p-type GaAs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Runtime</td>
<td>2.16 [sec]</td>
<td>8.36 [min]</td>
<td>0.46 [sec]</td>
<td>96.26 [min]</td>
</tr>
</tbody>
</table>
CHAPTER 5
NUMERICAL ISSUES

Summation

\[
\frac{C}{S} = \frac{q^2}{S \cdot h} \sum_{k_x, k_y} \int_{-\infty}^{\infty} dE T(E) F_r(E - \mu + \frac{h^2 (k_x^2 + k_y^2)}{2m_e})
\]  

(2-2)

\[
\frac{C}{S} = \frac{q^2}{h} \int_{-\infty}^{\infty} dE T(E) \left( - \frac{\partial f_{2D}(E)}{\partial E} \right)_{E=\mu}
\]  

(2-7)

Two conductance equations are used for n-type silicon. (2-2) includes summation and (2-7) is an analytical equation. The result from (2-7) could be considered to be a perfect answer and the result from (2-2) should be within an allowed error range (1%~3%) from the answer. To achieve high accuracy, summation interval and range are critical. \(k_x\) and \(k_y\) can be defined as follows.

\[
k_x = \frac{2\pi}{L_x} \cdot a, \quad k_y = \frac{2\pi}{L_y} \cdot b
\]  

(5-1)

where \(L_x\) and \(L_y\) are device length in x and y direction. \(a\) and \(b\) are integers. Let us assume \(L_x=L_y=L\) for simplicity. Then summation interval is

\[
\Delta k_x = \Delta k_y = \frac{2\pi}{L}
\]  

(5-2)

The summation range for \(k_x\) and \(k_y\) is assumed to be the same.

\[-m \leq a \leq m, \quad -m \leq b \leq m \]  

(5-3)

where \(m\) is an integer. \(m\) and \(L\) should be chosen carefully to guarantee high accuracy.

Function \(P(E,a,b)\) is defined as,

\[
T(E) F_r(E - \mu + \frac{h^2 (k_x^2 + k_y^2)}{2m_e}) = T(E) F_r(E, k_x, k_y) = P(E, a, b)
\]  

(5-4)

The summation and integration part of (2-2) is
\[
\sum_{a,b}^{\infty} dEP(E,a,b)
\]
\[
= \int_{-\infty}^{\infty} P(E,-m,-m)dE + \int_{-\infty}^{\infty} P(E,0,0)dE + \int_{-\infty}^{\infty} P(E,0,1)dE + \int_{-\infty}^{\infty} P(E,0,2)dE
\]
\[
+ \cdots + \int_{-\infty}^{\infty} P(E,m,m)dE
\]
(5-5)

\(P(E,a,b)\) has a form of hyperbolic secant function. With fixed \(E\), as the absolute value of \(a\) or \(b\) increases, \(P(E,a,b)\) decreases.

\[
|a| \to \infty \text{ or } |b| \to \infty, \quad P(E,a,b) \to 0 \quad E \text{ is fixed}
\]
(5-6)

An example of (5-6) is given in Fig. 5-1. \(m\) is chosen such that the maximum value of \(P(E,m,m)\) is less than 1% of that of \(P(E,0,0)\).

\(L\) is determined self-consistently. Sufficiently large value which is in an order of micrometers is chosen first. If the simulation data based on the first \(L\) is well matched with the data from the 2D Fermi function (n-type) or the experimental data (p-type), shorter \(L\) is chosen for the next simulation. \(L\) is reduced in this way until the runtime of the simulation is fast enough and the simulation data is within an allowed error range.

**Integration**

The adaptive Simpson algorithm is employed for integration [13]. Setting appropriate tolerance for the algorithm is crucial to guarantee not only high accuracy but also optimized runtime. If the tolerance is too tight, the algorithm would run for a long time. If the tolerance is too loose, error would be out of the allowed range. Moreover, machine precision should be taken into account. For instance, in the case where the machine precision is 4 digits and integral value has one digit after decimal point, the tolerance needs to be at least \(10^{-1}\). If the tolerance is less than or equal to \(10^{-2}\), a
computing machine would not be able to handle it. On the contrary, the tolerance could be too large and beyond the machine precision. Scale of the integral value should be considered, too. If the first non zero number of the integral value comes 2 digits after the decimal point, the tolerance should be less than or equal to $10^{-3}$. Otherwise, error would be significant (see Fig. 5-2).

The undesired examples mentioned above could take place when the Simpson algorithm with fixed tolerance is used for many integrands which have integral values over a large range. In this thesis, for example, p-type silicon conductance is simulated on ten different doping concentrations in a range from $1.6e18$ to $3e20$ and the biggest conductance is $10^6$ times larger than the smallest one.

In order to avoid the undesired examples, first, integral value, which is conductance, is estimated by using the experimental value. Constant $A$, is chosen such that the integral value divided by $A$ is in the order of zero. Next, input (integrand) to the Simpson algorithm is divided by $A$. Tolerance is set to be $10^{-4}$ (Tolerance can be fixed because $A$ is different for different integral values). Output is multiplied back by $A$. This treatment on the input and output guarantees that all of the integral values are within $10^{-4}$ error (see Fig. 5-3). When the experimental values are not available, we can run the algorithm with random tolerance first. The tolerance can be adjusted after based on the output of the first run.

**Poisson Equation**

$$-\frac{d}{dz} \left( \varepsilon_r \frac{dU}{dz} \right) = \frac{q^2}{\varepsilon_0} n(z)$$  \hspace{1cm} (2-13)
The Poisson equation has a form of a second order differential equation. The left hand side of (2-13) can be discretized using the finite difference method and it turns into a matrix form.

\[ [D][U] = c[N] \]  \hspace{1cm} (5-7)

where \([D]\) is a coefficient matrix, \([U]\) is potential, \(c\) is a constant, and \([N]\) is electron density matrix. \([U]\) could be found as,

\[ [U] = c[D]^{-1}[N] \]  \hspace{1cm} (5-8)

Inverting matrix is acceptable when the matrix size is small. But \([D]\) in this simulation has a size of double precision 1000 x 1000. Inverting \([D]\) would result in significant error and a waste of runtime and memory space. Basically, (5-7) is a linear equation and we can use L-U decomposition method instead. This method requires much less computation time and the error is negligible. In addition, \([D]\) is tridiagonal matrix and three arrays can be used to represent \([D]\). L-U decomposition is performed on the three arrays rather than the large matrix.
Figure 5-1. $P(E,a,b)$ decreases as the absolute value of $a$ or $b$ increases.
Figure 5-2. Three examples of inappropriate tolerance. A) Tolerance is too small and it is out of machine precision. Machine precision is assumed to be 4 digits. B) Tolerance is too big and it is out of machine precision. Machine precision is assumed to be 4 digits. C) Tolerance is within machine precision but it is so large that error would be significant.

Figure 5-3. Constant A is chosen to tune integral into the number in the order of zero. Input (integrand) is divided by A and the output is multiplied back by A. By using A, the fixed tolerance can be used for different integrands. The runtime is optimized and the error is always within 10^-4.
CHAPTER 6
CONCLUSION

The specific NiSi-nSi and NiSi-pSi contact resistances are simulated over a wide range of doping concentrations using the ballistic NEGF modeling method and the result is compared to the experimental data. The barrier height is fitted using the experimental data of the lowest or second lowest concentration. For n-type case, the numerical integration and 2D Fermi function approaches are compared and they show good agreement proving the numerical integration approach in this thesis has high accuracy. The investigation on accuracy of the numerical integration approach is essential for p-type case where 2D Fermi function cannot be employed. Due to lack of experimental data, simulation result of GaAs is compared with that of Si based on the fixed barrier height and concentration. For high concentration, n-type GaAs has higher resistance than n-type Si even though n-type GaAs has lighter effective mass. This is because n-type GaAs has only one mode and n-type Si has six modes. When the barrier width is so thin that all modes have high transmission, n-type Si can have lower resistance. p-type GaAs has always lower resistance than that of p-type Si because they have the same number of modes and the effective mass for p-type GaAs is lighter. Parallel computing is used for the simulation. For n-type Si algorithm, speedup has a peak value at 16 CPUs. The efficiency of the parallel algorithm drops quite rapidly. This is due to the fact that computation time is not large for this simulation. If the same algorithm is applied to other simulations where computation is expensive, the speedup would have a peak value at more than 16 CPUs and the efficiency would drop slowly.
APPENDIX
THE FORTRAN CODE FOR THE ADAPTIVE SIMPSON ALGORITHM

!adaptive Simpson algorithm
module quad_module
  implicit none
  contains
    subroutine quad(Q,fcnt,f,a,b,tol)
      implicit none
      ! integrand
      external::f  !the integrand
      ! integration range
      double precision,intent(in)::a,b
      ! absolute tolerance
      double precision,intent(in)::tol
      ! function count
      integer,intent(out)::fcnt
      ! return value
      double precision,intent(out)::Q

    ! local variable
    double precision::h,hmin,c,d,e
    double precision::x1,x2,x3,x4,x5,x6,x7
    double precision::y1,y2,y3,y4,y5,y6,y7
    double precision::Q1
    double precision::Q2
    double precision::Q3
    integer::warn
    integer::warn1,warn2,warn3

      fcnt=0
      h=0.13579*(b-a)
      x1=a
      x2=a+h
      x3=a+2*h
      x4=(a+b)/2
      x5=b-2*h
      x6=b-h
      x7=b

      call f(x1,y1)
      call f(x2,y2)
      call f(x3,y3)
      call f(x4,y4)
      call f(x5,y5)
      call f(x6,y6)
      call f(x7,y7)
fcnt=fcn+7

hmin=epsilon(b-a)/1024

call quadstep(Q1,fcnt,warn1,f,x1,x3,y1,y3,tol,hmin)
call quadstep(Q2,fcnt,warn2,f,x3,x5,y3,y5,tol,hmin)
call quadstep(Q3,fcnt,warn3,f,x5,x7,y5,y7,tol,hmin)

Q=Q1+Q2+Q3
warn = max(warn1,warn2,warn3)
end subroutine quad

recursive subroutine quadstep(Q,fcnt,warn,f,a,b,fa,fc,fb,tol,hmin)

implicit none
!

!   subroutine argument list
! external::f   !the integrand
!   integration range
! double precision,intent(in)::a,b
!   function value
! double precision,intent(in)::fa,fc,fb
!   absolute tolerance
! double precision,intent(in)::tol
! double precision,intent(in)::hmin
!   function count
integer,intent(inout)::fcnt
integer,intent(out)::warn
double precision,intent(out)::Q
!

!   local variable
integer::maxfcn
! double precision::h
double precision::c,d,e
! double precision::Q1,Q2
double precision::Qac,Qcb
double precision::fd,fe
integer::warnac,warncb
!

! maximum function count
maxfcn=9000
h=b-a
c=(a+b)/2
d=(a+c)/2
e=(c+b)/2
call f(d,fd)
call f(e,fe)
fcnt=fcnt+2
Q1 = (h/6)*(fa + 4*fc + fb);
Five point double Simpson's rule.
\[ Q_2 = \frac{h}{12} \times (f_a + 4 \times f_d + 2 \times f_c + 4 \times f_e + f_b); \]

One step of Romberg extrapolation.
\[ Q = Q_2 + \frac{(Q_2 - Q_1)}{15}; \]

termination criterion

floating point
if \( \text{abs}(Q) \geq \text{huge}(1.0) \) then
    warn=3
    print\(*\), 'floating point'
    return
end if

reached maximum function count
if (fcnt > maxfcnt) then
    warn=2
    print\(*\), 'reached maximum function count'
    return
end if

error is less than the tolerance
if \( \text{abs}(Q_2 - Q) \leq \text{tol} \) then
    warn=0
    print\(*\), 'error is less than the tolerance'
    return
end if

prevent infinite recursion
if ((\text{abs}(h) < hmin).OR.(c==a).OR.(c==b)) then
    warn=1
    print\(*\), 'infinite recursion'
    return
end if

call quadstep(Qac,fcnt,warncb,f,c,f,fd,fc,fe,fb,tol,hmin)
call quadstep(Qcb,fcnt,warncb,f,c,b,fc,fe,fb,tol,hmin)
Q=Qac+Qcb
warn=max(warncb,warncb)
end subroutine quadstep
end module quad_module
LIST OF REFERENCES


BIOGRAPHICAL SKETCH

Dukjin Kim was born in Kyungbuk, South Korea. He received his Bachelor of Science degree in electrical and computer engineering from Hanyang University–Seoul, South Korea in 2008. In 2009, he started his M.S. study in electrical and computer engineering under the guidance of Professor Jing Guo at the University of Florida–Gainesville, Florida. His research in the graduate school is focused on parallel simulation of silicide semiconductor contact resistance.