Impact of channel thickness on the relocation of valleys in nano Silicon and Germanium DG-MOSFETs with alternative wafer orientation

Morteza Charmi*

Nano Physics Department, Malek-Ashtar University of Technology, Shahinshahr, Isfahan, Iran

Abstract- In this paper, a detailed simulation study of the channel thickness on the relocation valleys in double gate germanium and silicon MOSFETs with alternative wafer orientation is presented. Quantum simulation is performed based on self-consistent solutions of 2D Poisson's equation and Schrodinger equation with a generalized effective mass approach, within the non-equilibrium Green's function formalism. The effects channel thickness on the relocation of valleys are studied by focusing on the maximum subband potential, subband occupancy, subthreshold swing and on current for alternative wafer orientation. The results illustrate that the channel thickness supplants the valleys and their occupations that lead to different value of on current for every wafer orientation.

Keywords: DG MOSFETs; non-equilibrium Green's function; channel thickness; wafer orientation; valleys.

PACS numbers: 72.10.Bg, 73.23.-b, 73.40.Qv, 73.43.Cd

*Corresponding author: E-mail: charmi.phy@gmail.com
Tel: 00989132135691, Fax: 00983125220605
I. INTRODUCTION

Long term research is focused on replacing charge-based electronics with spintronics, quantum computers, or optical computers [1, 2]. In the near term, researchers are looking for ways to continue improving traditional devices with alternative channel materials [3-6], different wafer orientation [7, 8], Strained channel [9-12] and structures such as nanotube or nanowire transistors [13, 14] that could outperform silicon CMOS. Recently, III-V materials and Germanium have generated a great deal of interest because of their high electron mobility. It is desired to use modeling and simulation techniques to determine how well these materials could perform in future technology generations compared to silicon [15, 16]. Under ballistic conditions, the main advantage of a semiconductor with a small transport mass is its high injection velocity. However, these materials also have a very low density of states in the $\Gamma$-valley, which tends to greatly reduce the inversion charge and hence reduce drive current [17-19].
The theoretical study of ballistic devices with new channel materials and various surface/transport orientations is a challenge because the effective mass tensor (EMT) becomes non-diagonal and the effective mass equations (EME) become complicated. Therefore it is desired to use a generalized effective-mass approach for simulation of n-type MOSFET on arbitrarily oriented wafers [20]. In this paper, the non-equilibrium Green’s function (NEGF) method and the effective mass equation have been used to describe the transport and quantization effects, with consideration of all valleys.

II. DEVICE STRUCTURE

A schematic picture of the double gate MOSFET structure is shown in Fig. 1. A gate length of 8 nm with body doping concentration of $10^{17} \text{ cm}^{-3}$, source/drain length of 7.5 nm, source/drain doping concentration of $2 \times 10^{20} \text{ cm}^{-3}$, equivalent oxide thickness EOT = 0.5 (high-k=20, $T_{\text{oxide}}=2.56$ nm) and power supply voltage, $V_D=0.6$ V are considered in this work. All parameters are according to the end of the international technology roadmap for semiconductors (ITRS-2013) [21]. It is worth noting that the off current was adjusted to a fixed value ($I_{\text{off}}=0.1 \mu\text{A/\mu m}$) by varying the gate work function for every
overdrive in this work. There is no source/drain doping gradient and the junctions are abrupt.

III. SIMULATION APPROACH

The effective mass equation (EME) is, easy to implement model Hamiltonian that does justice to the device bandstructure including quantum confinement effects within the inversion layer, and describes the slowly varying envelope part of the underlying Bloch wavefunction. The Non-Equilibrium Green’s Function (NEGF) method and the generalized effective mass equation have been used to describe transport in nanoscale MOSFETs. It is clear that the quantum simulation of Si (100) devices is substantially simplified by the fact that the principal axes of the six-fold degenerate conduction band ellipsoids are aligned along the device coordinate axes. In general, however, the principal axes of the conduction band ellipsoids are not aligned with the device axes, so that the associated kinetic energies become coupled and the effective mass equation (EME) becomes nontrivial. To extend the application of EME to analyze these novel n-MOSFETs and to contribute the multiple valleys, it is necessary to generalize the EME approach to arbitrary wafer orientations that was addressed in [20].
The 2D ballistic transport equation in the MOSFET channel region was solved by a mode space approach [22], which splits the problem into two 1D problems. In quantum confinement direction (the z-direction), the Schrödinger equation was solved to generate the subbands. In transport direction (the x-direction), the non-equilibrium Green’s function approach which is equivalent to solving the Schrödinger equation with the open boundary condition, was used to describe the ballistic quantum transport. The Schrödinger equation in the confinement direction and the non-equilibrium Green’s function in the transport direction are solved self-consistently with the 2D Poisson equation.

In the vertical direction (z-direction in Fig. 1), the Schrödinger equation was solved for each x-position independently to generate the ith subband profile, $E_i(x)$, and the corresponding wave function, $\psi_i(x, z)$:

$$
-\frac{\hbar^2}{2m_z^*} \frac{\partial^2}{\partial z^2} \psi_i(x, z) - qV(x, z)\psi_i(x, z) = E_i(x)\psi_i(x, z)
$$

where $m_z^*$ is the effective mass along z-direction, $q$ is the electron charge, $\hbar$ is the Planck’s constant, $V(x, z)$ is the electrostatic potential [23-25].

The retarded Green’s function for the device in matrix form is computed as:

$$
G(E) = \left[(E + i\eta)I - H - \Sigma_s - \Sigma_d\right]^{-1}
$$

where $\Sigma_s$ and $\Sigma_d$ are the self-energies of the source and drain, respectively, $\eta$ is an
infinitesimal positive value, \( E \) is the energy, \( I \) is the identity matrix, and \( H \) is the Hamiltonian of the mode space approach. As can be seen from Eq. (2), the transport is assumed here to be completely ballistic. The spectral density functions due to the source/drain contacts can be obtained as [23]:

\[
A_s = G \Gamma_s G^\dagger \quad \text{and} \quad A_D = G \Gamma_D G^\dagger
\]  

(3)

where \( \Gamma_s = i(\Sigma_s - \Sigma_s^\dagger) \) and \( \Gamma_D = i(\Sigma_D - \Sigma_D^\dagger) \). The source related spectral function is filled up according to the Fermi energy in the source contact, while the drain related spectral function is filled up according to the Fermi energy in the drain contact and diagonal entries of spectral functions, represent the local density-of-states at each node [23]. In the longitudinal direction, the non-equilibrium Green’s function (NEGF) approach was used to describe the ballistic, quantum transport. The 2D electron density is:

\[
n_{2D}(x) = \sum_i \left\{ \int_{-\infty}^{+\infty} dE [F_{-1/2}(\mu_s - E)D_{SI}(E,x) + F_{-1/2}(\mu_D - E)D_{DI}(E,x)] \right\}
\]

(4)

where \( F_{-1/2} \) is the Fermi integral of order \(-1/2\) [26], \( \mu_s(\mu_D) \) is the source/drain Fermi level, and \( D_{SI}(E,x) \) (\( D_{DI}(E,x) \)) is the local density of states (LDOS) of the ith subband contributed by the source (drain), which is calculated based on the Green’s function formalism. The 2D electron density, \( n_{2D}(x) \), is then weighted by the eigenfunction at the position \( x, \psi_i(x,z) \), to get the 3D electron density:

\[
n_{3D}(x,z) = n_{2D}(x)|\psi_i(x,z)|^2
\]

(5)
A 2D Poisson equation was then solved in the silicon channel and gate oxide to update the electrostatic potential (A nonlinear Poisson equation was solved to improve the outer loop convergence [27]). The iteration between the quantum transport equation and the Poisson equation was repeated until the self-consistency was achieved. Finally the source-drain current can be calculated [23]:

\[
I_{SD} = \sum_i I_{0i} \int_{-\infty}^{\infty} \left[ F_{-\frac{1}{2}}(\mu_s - E) - F_{-\frac{1}{2}}(\mu_D - E) \right] T_{SDi}(E) dE
\]  

(6)

where \( I_{0i} \) is a constant with the dimension of current, \( F_{-\frac{1}{2}} \) is the Fermi-Dirac integral of order \(-\frac{1}{2}\), \( \mu_{S/D} \) is the source/drain Fermi level, the index of \( i \) is the number of subbands and \( T_{SDi} \) is the transmission coefficient from the source to drain for the \( i \)th subband at energy \( E \):

\[
T(E) = \text{trace} \left( \Gamma_s(E) G(E) \Gamma_d(E) G^\dagger(E) \right)
\]  

(7)

### IV. RESULTS AND DISCUSSION

In this work, I study the Si and Ge DG MOSFET with alternative wafer/transport/width orientation such as \((001)\|/[100]/[010]\), \((110)\|/[1\bar{1}0]/[001]\) and \((111)\|/[\bar{2}11]/[0\bar{1}0]\), that here the first, second and third sets of indices specify the wafer orientation (quantum confinement direction), the transport direction (x direction) and width (y direction), respectively. Some work has shown that using the bulk effective
masses is reasonably accurate for silicon and germanium ultrathin body (UTB) n-MOSFETs with different crystal orientations and in most cases, the validity of the parabolic effective mass approximation (EMA) is quite satisfactory [28]. While for analyses of III-V ultra-thin MOSFETs the bulk effective mass leads to significant errors and never be used, therefore a rigorous treatment of full band structure is required [15]. The bulk effective masses used into the device coordinate system for every valley and alternative wafer direction are summarized in table 1. The confinement direction is considered as the Z coordinate, thus $m_z$ is the quantization mass, $m_x$ is transport mass and $m_y$ is the effective mass along the width of the DG MOSFET, $g_0$ is the degeneracy of each set of valleys, $g_{\text{offset}}$ is the valley energy offset with respect to lowest valley and $m_d$ is the density-of-states effective mass per valley that can be readily obtained from the expression, $m_d = \sqrt{m_x m_y}$ [20].

Fig. 2 shows the maximum of potential energy profile (potential at the top of the barrier), for ultra-thin double gate germanium and silicon MOSFETs with alternative wafer orientation, versus channel thickness. The maximum potential energy (the potential energy at the top of the potential barrier) is plotted separately for each valley. The increase of the confinement effective mass (the effective mass in $z$ direction) for each valley, causes the electrons first occupy that valley, thus, the potential barrier in
comparison with other valleys is decreased. For example in Fig. 2 for Si(001), according to table 1 the effective mass of $m_z$ for $X_1$ valley is greater than it’s amount for $X_2$ and $X_3$ valleys so the potential barrier of $X_1$ valley is less than others and at first the $X_1$ valley is occupied. For Si(110) the same approach is occurred. But for Si(111) the confinement effective mass for $X_1$ valley and $X_2$ valley is identical, so the potential barrier is the same for both valleys. About the Ge(001), the $X_1$ valley has the greatest $m_z$ and the less potential, the $\Gamma$ valley has the least $m_z$ and the greatest potential barrier. Moreover for Ge(110) the $X_2$ valley has the greatest confinement effective mass, so it has the minimum potential energy. It means that, at first, this valley is occupied by electrons. Finally for Ge(111), the $L_1$ valley has the greatest $m_z$ and the least potential.

Fig. 3 indicates the percentage of electron subband occupation versus the channel thickness. The most portion of the electron current in lower channel thickness (maximum quantum confinement) is related to the valleys with the higher confinement effective mass. By increasing the channel thickness the most portion of the electron current almost tends to the valleys with minimum conduction bands of the bulk effective mass. For Si(001) the all electron current in lower thickness is related to the $X_1$ valley that has the lower potential barrier than other subbands. By increasing the channel thickness to 5 nm, $X_1$ valley’s share current, decrease to 60%; $X_2$ and $X_3$ valley’s share, increase to 10% and
30% respectively. For Si(110) all the currents is almost from the X₂ valley, that has fourfold degeneracy and larger confinement effective mass. The percent of electron subband occupation for both valleys in Si(111) is identical. About the Ge(001) with 1 nm thickness, the X₁ valley has the most portion of the electron current and in higher channel thickness the most current is from the L valley. For Ge(110), at first all the current is from the X₂ valley then with increasing the thickness to 5 nm all the current is supplied by L₁ valley. Finally for Ge(111), all of the current, with any channel thickness is related to the L₁ valley, because this valley has the most confinement effective mass and has the less potential barrier. Moreover with increasing the channel thickness, the quantum confinement effects are getting lower and bulk properties are salient, so the most occupation percentage tends to the bulk germanium minimum conduction band, which is the L valley.

It should be noted that the off current was adjusted to a fixed value (I_{off}=0.1 \mu A/\mu m) for every overdrive in this work. Fig. 4 shows the on current at V_{GS}=V_{DS}=V_{DD}=0.6 V for ultra-thin double gate germanium and silicon MOSFETs with alternative wafer orientation, versus channel thickness. In channel thickness of 1 nm, Si(110) and Ge(110) have the maximum on current, because in 1 nm thickness, only X₂ valley of Si(110) and X₂ valley of Ge(110) are occupied. Which according to the table 1 these two valleys have
fairly high and identical density of state mass ($m_d$), also potential barrier is small for these two valleys (Fig. 2). Therefore in channel thickness of 1 nm Si(110) and Ge(110) have the maximum on current. The minimum on current in 1 nm thickness is related to Ge(111), because the L$_1$ valley which has the all current occupation, has the less density of state mass. Si(111), Si(001) and Ge(001) have been mediocre on current for 1 nm thickness. In channel thickness of 3 nm Ge(110) has the 5$^{th}$ value of on current while in thickness of 1 nm it has the most value of on current. Because in thickness of 3 nm, 70% of the current is due to L$_1$ valley and 30% of the current is due to X$_2$ valley.

With increasing the channel thickness, the most percentage of current tends to the valleys with the minimum bulk conduction band. It means that for germanium, with increasing the channel thickness, the maximum subband occupancy is related to the L valley, which is the minimum bulk conduction band of germanium. Furthermore, with increasing the channel thickness the inversion charge in the channel is reduced, and leads to the reduction in on current which is well characterized in Fig. 4. The minimum on current for all channel thickness is related to Ge(111), because for any thickness only the L$_1$ valley is occupied which has the minimum density of state mass.
Fig. 5 shows the dependence of the subthreshold swing on the channel thickness. It is clear that with increment of the channel thickness, due to decrease of the gate control on the channel, the subthreshold swing is increased. For Ge(111) that have the smallest on current value, have the biggest subthreshold swing value than the others. Of course due to small channel length ($L_g = 8$ nm) to the channel thickness ratio, the values of $S$ parameter are large. In channel thickness larger than 2 nm, for all different wafer orientation of Ge and Si, the $S$ parameter is almost larger than 80 mV/decade which is not suitable for a well-designed MOSFET (the $S$ parameter for a well-designed MOSFET is less than 80 mV/decade[25]).

As mentioned before, the off current was adjusted to a fixed value ($I_{off} = 0.1 \mu A/\mu m$) for every overdrive in this work. So the gate work-function become a variable parameter to obtain a fixed off current. Therefore the plot of gate work-function versus channel thickness for alternative wafer orientation of Si and Ge is shown in Fig. 6. According to the table 1, the Ge(111) that has the smallest density of state ($m_d$) and the smallest transport effective mass ($m_x$), has the largest gate work function than the others. In the off-current state due to small $m_x$, the tunneling current from source to drain, is increased and leads to increase of the off current. But for fixed value of off current, this increasing must be compensated by increase of the gate work-function that is clear in Fig. 6. Moreover by
increment of $T_{ox}$ the off current is increased and for fixed $I_{off}$ a higher gate work-function is needed.

It is worth noting that in ultra-thin DG MOSFETs, by decrease of the channel thickness the gate quantum confinement effect is increased. So the subbands energy at the top of the potential barrier and the percentage of subbands occupancy are supplanted for every valley orientations. So the channel thickness is the important parameter that should be considered. In addition it is clear that in ultra-thin DG MOSFETs, for any wafer orientations, the current is variable for any channel thickness and every valley can participate in the on current. While in the bulk MOSFETs only the bulk conduction minimum band is occupied and the current is only proceed of this valley.

V. CONCLUSION

The impacts of channel thickness on the relocation of valleys in double gate germanium and silicon MOSFETs with alternative wafer orientation have been studied. The simulation is based on the non-equilibrium Green’s function method within generalized effective mass formalism. The maximum subband potential, the percent of subband occupancy, on current, subthreshold swing and the effective mass for every valley have been investigated. The results show that, in ultra-thin DG MOSFETs, by varying the
channel thickness, the valleys are supplanted and the on current can be due to every valley (not only minimum conduction band valley). Moreover the percent participation of each valley on the output current is different and is dependent on the channel thickness.
VI. REFERENCES


Table Captions

Table 1  Effective mass information used into the device coordinate system for every valley and wafer orientation

Figure Captions

Figure 1  Schematic cross-sectional view of ultra-thinDG-MOSFET.

Figure 2  Maximum potential energy profile (the potential energy at the top of the potential barrier) for ultra-thin double gate germanium and silicon MOSFETs with alternative wafer orientation by consideration of all valleys, versus channel thickness.

Figure 3  Electron subband occupation for ultra-thin double gate germanium and silicon MOSFETs with alternative wafer orientation by consideration of all valleys, versus channel thickness.

Figure 4  On current for ultra-thin double gate germanium and silicon MOSFETs with alternative wafer orientation, versus channel thickness.

Figure 5  Subthreshold swing for ultra-thin double gate germanium and silicon MOSFETs with alternative wafer orientation, versus channel thickness.

Figure 6  Gate workfunction for ultra-thin double gate germanium and silicon MOSFETs with alternative wafer orientation, versus channel thickness.
<table>
<thead>
<tr>
<th>Material</th>
<th>Valley</th>
<th>$g_x$</th>
<th>$m_x$</th>
<th>$m_y$</th>
<th>$m_z$</th>
<th>$g_{z offset}$</th>
<th>$m_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>$X_1$</td>
<td>2</td>
<td>0.19</td>
<td>0.19</td>
<td>0.91</td>
<td>0</td>
<td>0.19</td>
</tr>
<tr>
<td></td>
<td>$X_0$</td>
<td>2</td>
<td>0.19</td>
<td>0.91</td>
<td>0.19</td>
<td>0</td>
<td>0.416</td>
</tr>
<tr>
<td></td>
<td>$X_3$</td>
<td>2</td>
<td>0.91</td>
<td>0.19</td>
<td>0.19</td>
<td>0</td>
<td>0.416</td>
</tr>
<tr>
<td>Si</td>
<td>$X_4$</td>
<td>2</td>
<td>0.19</td>
<td>0.91</td>
<td>0.19</td>
<td>0</td>
<td>0.416</td>
</tr>
<tr>
<td>(110)/[1\bar{1}0]/[001]</td>
<td>$X_2$</td>
<td>4</td>
<td>0.55</td>
<td>0.19</td>
<td>0.314</td>
<td>0</td>
<td>0.32</td>
</tr>
<tr>
<td>Si</td>
<td>$X_4$</td>
<td>2</td>
<td>0.67</td>
<td>0.19</td>
<td>0.4</td>
<td>0</td>
<td>0.357</td>
</tr>
<tr>
<td>(111)/[\bar{2}11]/[0\bar{1}0]</td>
<td>$X_2$</td>
<td>4</td>
<td>0.23</td>
<td>0.55</td>
<td>0.4</td>
<td>0</td>
<td>0.356</td>
</tr>
<tr>
<td>Ge</td>
<td>L</td>
<td>4</td>
<td>0.149</td>
<td>0.6</td>
<td>0.117</td>
<td>0</td>
<td>0.299</td>
</tr>
<tr>
<td></td>
<td>$\Gamma$</td>
<td>1</td>
<td>0.038</td>
<td>0.038</td>
<td>0.038</td>
<td>0.14</td>
<td>0.038</td>
</tr>
<tr>
<td>Ge</td>
<td>$X_3$</td>
<td>2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.95</td>
<td>0.19</td>
<td>0.2</td>
</tr>
<tr>
<td>(001)/[100]/[010]</td>
<td>$X_2$</td>
<td>2</td>
<td>0.2</td>
<td>0.95</td>
<td>0.2</td>
<td>0.19</td>
<td>0.436</td>
</tr>
<tr>
<td></td>
<td>$X_3$</td>
<td>2</td>
<td>0.95</td>
<td>0.2</td>
<td>0.2</td>
<td>0.19</td>
<td>0.436</td>
</tr>
<tr>
<td>Ge</td>
<td>L</td>
<td>4</td>
<td>0.082</td>
<td>0.585</td>
<td>0.223</td>
<td>0</td>
<td>0.219</td>
</tr>
<tr>
<td></td>
<td>$L_2$</td>
<td>2</td>
<td>0.223</td>
<td>0.585</td>
<td>0.082</td>
<td>0</td>
<td>0.361</td>
</tr>
<tr>
<td></td>
<td>$\Gamma$</td>
<td>1</td>
<td>0.038</td>
<td>0.038</td>
<td>0.038</td>
<td>0.14</td>
<td>0.038</td>
</tr>
<tr>
<td>Ge</td>
<td>$X_4$</td>
<td>4</td>
<td>0.2</td>
<td>0.95</td>
<td>0.2</td>
<td>0.19</td>
<td>0.436</td>
</tr>
<tr>
<td>(110)/[1\bar{1}0]/[001]</td>
<td>$X_3$</td>
<td>2</td>
<td>0.575</td>
<td>0.2</td>
<td>0.33</td>
<td>0.19</td>
<td>0.339</td>
</tr>
<tr>
<td>Ge</td>
<td>L</td>
<td>1</td>
<td>0.08</td>
<td>0.08</td>
<td>1.64</td>
<td>0</td>
<td>0.08</td>
</tr>
<tr>
<td></td>
<td>$L_2$</td>
<td>1</td>
<td>1.467</td>
<td>0.08</td>
<td>0.089</td>
<td>0</td>
<td>0.343</td>
</tr>
<tr>
<td></td>
<td>$L_3$</td>
<td>2</td>
<td>0.105</td>
<td>1.12</td>
<td>0.089</td>
<td>0</td>
<td>0.343</td>
</tr>
<tr>
<td>Ge</td>
<td>$X_4$</td>
<td>2</td>
<td>0.7</td>
<td>0.2</td>
<td>0.271</td>
<td>0.19</td>
<td>0.374</td>
</tr>
<tr>
<td>(111)/[\bar{2}11]/[0\bar{1}0]</td>
<td>$X_2$</td>
<td>4</td>
<td>0.243</td>
<td>0.575</td>
<td>0.271</td>
<td>0.19</td>
<td>0.374</td>
</tr>
</tbody>
</table>
Figure 1
Figure 3
Figure 4

On Current [μA/μm] vs. Channel Thickness [nm] for different materials and orientations:

- Si (001)/(110)/[010]
- Si (110)/(1-10)/[001]
- Si (111)/(1-211)/[0-11]
- Ge (001)/(100)/[001]
- Ge (110)/(1-10)/[001]
- Ge (111)/(1-211)/[0-11]

Parameters:
- $V_{ds} = V_{gs} = V_{in} = 0.6$ V
- $I_{off} = 0.1$ μA/μm
Figure 5
Figure 6