Quantum Mechanical Simulation in DG MOSFETs Based on a Tight Binding Green's Function Formalism

M. Ogawa, N. Kagotani, M. Ohta, and T. Miyoshi

Department of Electrical and Electronics Engineering,
Kobe University
1 Rokkodai, Nada, Kobe, 657-8501, Japan
ogawa@eedept.kobe-u.ac.jp

Abstract

We report studies of quantum transport in double gate Si MOSFETs (DG MOSFETs) based upon a full-2D tight-binding Green's function method. As a result, it is found that the I-V characteristics is quite different when a realistic band structure with 6 valleys is taken into account compared with the case of isotropic effective mass. More importantly, it is also found that the carriers flow not only in the lowest subband but also the second lowest one around the drain region, which cannot be expressed in conventional quantum correction methods.

1 Introduction

As rapid progress in MOS device scaling continues, channel lengths as short as 5 nm have already been achieved. The MOS scaling less than sub-10 nm gate length has revealed crucial issues such as the degradation of sub-threshold characteristics and source to drain (S-D) tunneling due to the quantum effects. Detailed physical simulations play important role in the understanding and development of such nano-scale MOSFET technology. So far, quantum correction models [1] have been applied to analyze such problems. In this paper, we report the results of full-2D quantum mechanical simulation based on a Green's function formalism in order to understand these issues more physically. In the simulation, both the two-dimensional quantum transport equation and the Poisson's equation are analyzed simultaneously taking into account the realistic band structures of Si. The simulation results with the anisotropic effective masses and with an isotropic effective mass are compared. The results for two different approaches, that is, real-space approach and mode-space solution are also compared.

2 Theory

The simulated double gate (DG) MOSFET device structure is shown in Fig. 1(a). A uniform discretization scheme is adopted for the 2D real-space approach in both x and y directions with mesh spacing Δ_x and Δ_y, respectively. Assuming the band structure of Si is comprised of equivalent 6 ellipsoides as shown in Fig. 1(b), the Hamiltonian of valley v $(= 1, 2, 3; 1', 2', 3')$ is

$$H_v = -\frac{1}{2}\left[\frac{\partial}{\partial x}\left(\frac{1}{m_x^v}\frac{\partial}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{1}{m_y^v}\frac{\partial}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{1}{m_z^v}\frac{\partial}{\partial z}\right)\right] + U(x, y), \tag{1}$$

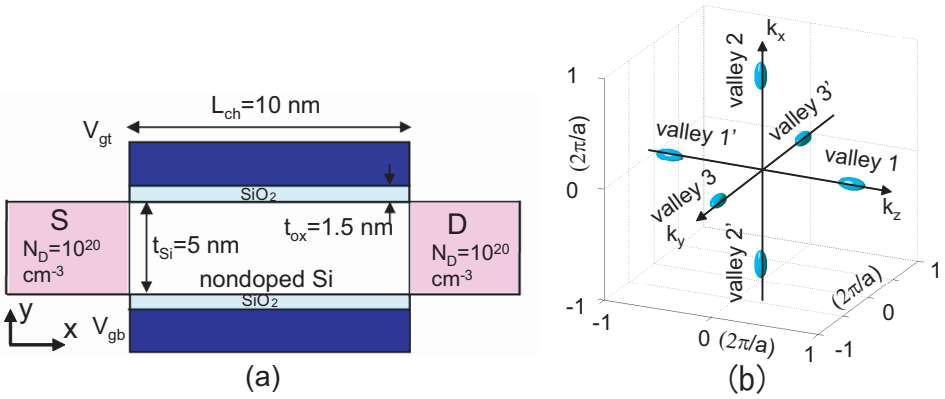

Figure 1: (a)Schematic structure of a DGMOSFET under investigation. $L_{\rm gtop} = L_{\rm gbot} = 10$ nm, $t_{\rm Si} = 5$ nm, $t_{\rm ox} = 1.5$ nm, $N_{\rm D} = 1.0 \times 10^{20}$ cm^{-3} are assumed. (b)6 rotated ellipsoides in Si band structure.

where m_x^v, m_y^v, and m_z^v are the components of the effective mass in the valley v, and $U(x, y)$ is the potential. Since the channel is confined in the y direction, in the mode space approach [3], we can use eigenmodes in the y direction as basis functions rather than real space discretization. We have to note, however, that in the mode space approach the couplings among modes in the neighboring segments (i_x and $i_x \pm 1$) are completely neglected. In either approach, the retarded Green's function G is obtained from the following equation for each electron energy.

$$G = [EI - H - \Sigma_{\rm S} - \Sigma_{\rm D}]^{-1}\,, \tag{2}$$

where $\Sigma_{\rm S}$ and $\Sigma_{\rm D}$ are the appropriate boundary self-energies at the source and drain electrode, respectively. Carrier concentration is then given by

$$n(x, y) = \int \frac{dE}{2\pi} \left[A_{\rm S} f_{\rm FD}(\mu_{\rm S}, E) + A_{\rm D} f_{\rm FD}(\mu_{\rm D}, E)\right], \tag{3}$$

where $f_{\rm FD}$ is the Fermi-Dirac distribution function, $\mu_{\rm S/D}$ are the Fermi energies and $A_{\rm S/D}$ are the local density of states or spectral function at S/D electrodes defined as $A_{\rm S/D} = G(-2\mathbf{Im}\Sigma_{\rm S/D})G^\dagger \equiv G\Gamma_{\rm S/D}G^\dagger$. The transmitted current is given by

$$I = -\frac{q}{h}\int dE\, T(E)\left[f_{\rm FD}(\mu_{\rm S}) - f_{\rm FD}(\mu_{\rm D})\right], \tag{4}$$

where $T(E)$ is the transmission coefficient which can be expressed in terms of the Green's function as $T(E) = \mathbf{Tr}(\Gamma_{\rm S} G \Gamma_{\rm D}) G^\dagger$.
Poisson's equation, carrier concentration, and the transport equation are solved iteratively until a certain convergence criterion is satisfied to obtain the characteristics of the device.

3 Results and Discussion

Figure 2(a) shows the I-V characteristics taking account of the realistic band structure of Si with anisotropic effective masses compared to those with a single equivalent effective mass. It is found that these characteristics are significantly different, since most of the current is comprised of the carriers in the valleys 3-3', which have the heavy effective mass m_l in the confinement direction and light m_t in the propagation direction. The effect of non-saturation of the drain current, which is one of the peculiar short channel effects (SCEs) in nano-MOSFETs, is reduced due to the anisotropicity of the effective masses. Although valleys 1-1$'$ and 2-2$'$ have same effective masses in y direction (confinement direction), the effective masses are different in the transport direction, which causes the difference of the current concentration.
Figure 2(b) compares the real-space solution and the mode-space solution. Although the real-space solution takes into account all couplings with neighboring sites, the mode-space solution completely neglects the coupling of modes among the neighboring segments. Therefore, the decoupled mode-solution often shows inaccurate results as shown in Fig. 2(b). To avoid the inaccuracies, we have to take the mode coupling among the segments when the vertical potential profile changes drastically.

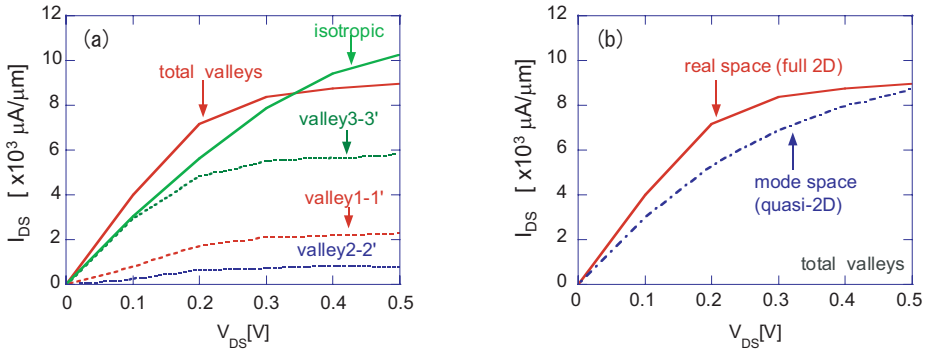

Figure 2: (a)I-V characteristics taking account of the anisotropic effective masses (total valleys) compared to those with an isotropic effective mass (isotropic).(b)Comparison of I-V characteristics of the real-space solution (solid line) with the mode-space solution (dashed line). ($V_{\rm gt} = V_{\rm gb} = 1.0$ V).

Figure 3(a) shows local density of states in the DGMOSFET. Several quasi-bound states are seen in the device. In the second subband, innegligible amount of carriers are existing. Tunneling through the potential barrier at the source end and quantum interference in the device are clearly observed. The label "2 fold" stands for valleys 3-3$'$ which have heavy effective mass in the confinement direction. Carriers flow not only in the lowest subband but also the second lowest one around the drain region, which cannot be expressed in conventional quantum correction methods.
Figure 3(b) shows the energy spectrum and its component in each valley of the current density flowing in the device. Valley 3-3$'$ stands for the component of the current through these valleys and so forth. As stated, current flows not only through the 1st subband of the valley 3-3$'$, but also through the 2nd subband. The amount of the carri-

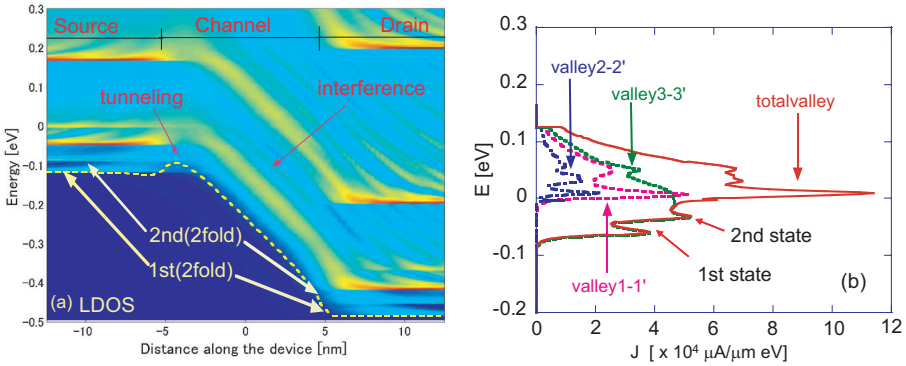

Figure 3: (a)Local density of states in the device under $V_{\rm gt} = V_{\rm gb} = 1.0$ V and $V_{\rm ds} = 0.4$ V. "2 fold" stands for valleys 3-3′ which have heavy effective mass in the confinement direction whereas light effective in the transport direction. (b)Energy spectrum of the current density. The 1st and 2nd subbands indicated by arrows are those of the 2 fold valleys.

ers in the higher level is around 10 %, which cannot be neglected in the evaluation of MOSFET performances.

4 Conclusion

We have shown the results of full-2D quantum mechanical simulation based on a Green's function formalism in order to understand some issues inherent to nano-MOSFETs. In the simulation, both the two-dimensional quantum transport equation and the Poisson's equation are analyzed simultaneously taking into account the realistic band structures of Si.

The simulation results with the anisotropic effective masses and with an isotropic effective mass are compared. The I-V characteristics are found significantly different since most of the current is comprised of the carriers in the valleys 3-3', which have the heavy effective mass in the confinement direction, that is, the anisotropic effective masses significantly affect the transport characteristics.

The results for the real-space approach and mode-space solution are also compared. We have to take the mode coupling among the segments when the vertical potential profile changes drastically.

The current flows not only through the ground subband but also through the higher subbands, which would affect the performance of the nano-scale MOSFETs.

References

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