

# 行政院國家科學委員會專題研究計畫 期中進度報告

次 32 奈米 CMOS 元件可靠性分析，量子結構效應，與蒙地  
卡羅電荷傳輸模擬(第 2 年)  
期中進度報告(精簡版)

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**Sub-32nm CMOS Device Reliability, Quantum Structure Effects and  
Carrier Transport Simulation by Using a Monte Carlo Method (2/3)**

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主持人：汪大暉 交通大學電子工程系教授

**中文摘要**

吾人利用 Luttenger-Kohn 模型計算次價電帶結構，自洽求解薛丁格及泊松方程式，應用於銻通道之雙閘極金氧半電晶體。此外，利用蒙地卡羅(Monte Carlo)方法模擬電洞傳輸特性求得電洞遷移率。由模擬結果得知，銻通道因為具有較低之傳導有效質量，所以具較高之電洞遷移率。此外，量子效應使得電洞遷移率在某個通道厚度下可被提升。

**Abstract**

The role of quantum confinement effect on hole mobility as a function of body thickness in Ge-channel DG-pMOSFETs is explored by solving the Boltzmann transport equation using the Monte Carlo method. The results show that the hole mobility of sub-20nm thickness exceeding the universal mobility can be achieved. This is attributed to an optimization of intrasubband and intersubband scattering rates.

**Keywords:** Luttinger-Kohn, Germanium, Double-gate, Monte Carlo simulation, hole mobility

**I. Introduction**

Double-gate (DG) metal oxide semiconductor field effect transistors (MOSFETs) and fin field effect transistor (FinFET) have been considered as the promising alternatives to the bulk MOSFETs in 22nm technology node and beyond [1-3] due to its immunity to short channel effect. In addition, advanced channel materials with high mobility compared to bulk Si, such as Ge [4] and III-V materials [5], also attract much attention to enhance device performance. Recently, experimental works have reported the possibility that the inversion carrier mobility can be further improved in quantum structure MOSFETs due to a subband modulation.[6-7] However, there has been little work on Ge-channel DG-pMOSFETs addressing the role of quantum confinement effect. On the other hand, as Lundstrom has pointed out [8], the channel backscattering coefficient plays an important role in determining the current drive and is strongly related to the near equilibrium mean free path, which can be extracted from a low-field mobility. As a consequence, it is crucial to explore the carrier transport properties in a scaled quantum device when an advanced channel material is used. It also can be

anticipated that the carrier scattering rate exhibits a dependence on a wavefunction distribution and a subband energy dispersion, which is varied significantly with the geometry of the quantum devices. In this work, we, therefore, analyze the quantum confinement effect on hole mobility versus body thickness ( $T_{Ge}$ ) in Ge-channel DG-pMOSFETs. The low-field hole mobility is calculated by a Monte Carlo method and only phonon scattering is present. The quantum confinement effect on hole mobility in Ge-channel is compared with Si-channel.

## II. Physical Model and Simulation Technique

Instead of one-mass approximation, the valence subband structures for the two-dimensional (2D) hole gas in Ge-channel DG-pMOSFETs are obtained self-consistently from the coupled Poisson and Schrödinger equations with a six-band Luttinger-Kohn Hamiltonian including spin-orbit-coupling [9]. On the other hand, the Bir-Pikus deformation potentials [10] are included to take into account the stress effect. The wavefunctions are set to zero in the Ge and gate dielectric interface, assuming that the wavefunctions do not penetrate the gate dielectric. In addition, an appropriate rotation matrix must be performed when dealing with the surface orientation other than the (100). The material parameters for both Si and Ge, including Luttinger parameters, deformation potentials, used in the calculation are given in Table I [11]-[13], respectively. Based on the calculated valence subband structures, a Monte Carlo method is then carried out to solve the Boltzmann transport equation to

compute the low-field mobility. Two relevant scattering mechanisms, acoustic phonon scattering and optical phonon scattering, are considered in the simulation.

Table I. The relevant material parameters and scattering parameters used in the Monte Carlo simulation for Si and Ge, respectively. The  $\gamma_1, \gamma_2$  and  $\gamma_3$  are Luttinger parameters and  $\Delta$  is the split-off energy. The  $a_v, b$ , and  $d$  are the Bir-Pikus deformation potentials. The  $C_{11}$  and  $C_{12}$  are elastic constants. The  $\Xi$  and  $D_iK$  are the average acoustic and optical deformation potential, respectively. The  $\hbar\omega$  is the phonon energy.

Material parameters									
	$\gamma_1$	$\gamma_2$	$\gamma_3$	$\Delta$ (eV)	$a_v$ (eV)	$b$ (eV)	$d$ (eV)	$C_{11}$ (dyn/cm <sup>2</sup> )	$C_{12}$ (dyn/cm <sup>2</sup> )
Si	4.285	0.339	1.446	0.044					
Ge	13.38	4.24	5.69	0.297	2.0	-2.2	-4.4	1.2853×10 <sup>12</sup>	4.826×10 <sup>11</sup>
Scattering parameters									
	$\Xi$ (eV)	$D_iK$ (10 <sup>8</sup> eV/cm)	$\hbar\omega$ (meV)						
Si	9.2	13	62						
Ge	11	6	38						

The relaxation time approximation is used, such that scattering process can be assumed to be either vector randomizing or isotropic elastic. The formulation of the scattering mechanisms can be found in [14-15] and are described briefly as follows. The acoustic phonon scattering rate is give by

$$S_{ac} = \frac{2\pi k_B T \Xi^2}{\hbar \rho u_1^2} \cdot D_n(E) \cdot H_{mn}(k_{\parallel}, k'_{\parallel})$$

where  $\Xi$  is the effective acoustic deformation potential,  $\rho$  is the material density,  $u_1$  is the sound velocity,  $T$  is lattice temperature and  $D_n(E)$  is the two dimensional density of hole states in  $n$ -th subband.

The optical phonon scattering rate is

$$S_{op} = \frac{\pi (D_iK)_{op}^2}{\rho \omega_{op}^2} \cdot [n_{op} + \frac{1}{2} \mp \frac{1}{2}] \cdot D_n(E \pm \hbar\omega_{op}) \cdot H_{mn}(k_{\parallel}, k'_{\parallel}) \\ \times \frac{1 - f_0(E \mp \hbar\omega_{op})}{1 - f_0}$$

where  $f_0$  is the Fermi-dirac distribution.  $D_iK$  is the average optical deformation potential  $n_{op}$  is

the Bose-Einstein distribution. The + and – represents the absorption and emission rates.

In the Monte Carlo simulation, a look-up table of the  $E-k$  relationship for the valence subbands is established. Only eigenvalues for  $k_{\parallel} < 0.6\pi/a_{\text{Ge}}$ , which significantly contribute to a low-field mobility, are evaluated. A single particle Monte Carlo simulation is performed under an external electric field. The simulation procedure is continued until the fluctuation in mobility due to the statistical error is less than 0.5%.

### III. Simulation Result

First of all, it should be pointed out that we use the calibrated scattering parameters of Si from a conventional Si-MOSFET and Ge from a SiGe-on-insulator device [16]. Fig. 1 shows the simulated device structure and corresponding inversion hole distribution.

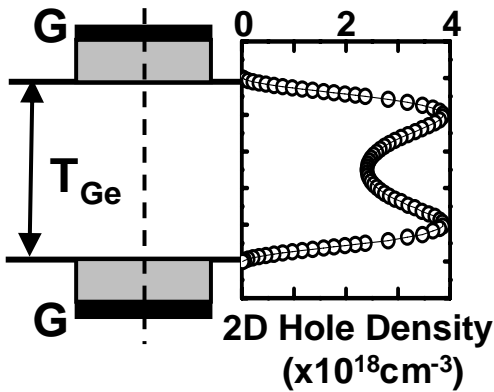


Fig. 1 Inversion hole distribution in a Ge-channel DG-pMOSFET.

Fig. 2 shows the simulated hole mobility versus body thickness in (100)/<010> Si-channel DG-pMOSFETs, where () and <> are the notations of surface orientation and channel direction, respectively. It is obvious that the hole

mobility decreases monotonically with body thickness. The simulation shows similar trend with the recent experimental data [6]. However, unlike in (100) Si-channel DG-pMOSFETs, the hole mobility as a function of body thickness in Ge-channel shows an enhancement characteristic.

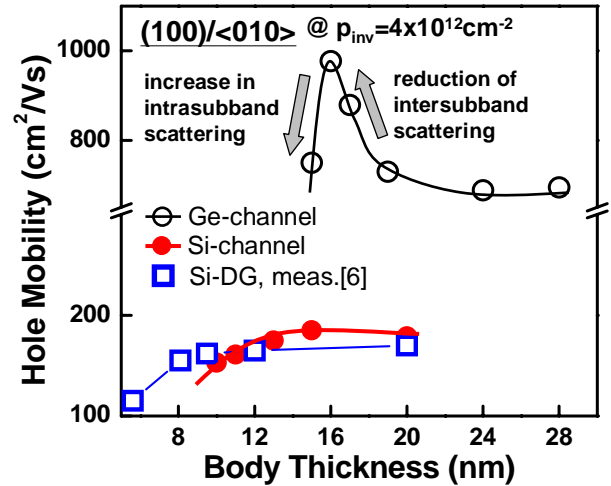


Fig. 1 Hole mobility as a function of body thickness for (100)/<010> Si- and Ge-channel DG-pMOSFETs. Only acoustic phonon and optical phonon scatterings are considered. The hole mobility enhancement is observed at a small body thickness. Note that the peak of hole mobility for Ge-channel is estimated to be about four times as large as for Si-channel.

When a body thickness is scaled down, the hole mobility increases gradually to a maximum around  $T_{\text{Ge}}=16\text{nm}$ , and then decreases drastically. Note that the calculated hole mobility at  $T_{\text{Ge}}=28\text{nm}$  is about  $700\text{ cm}^2/\text{Vs}$ , which significantly deviates from the bulk value of Ge. Thus, we examine the hole mobility in a very low  $p_{\text{inv}}$  where it is expected to recovery the bulk mobility. However, the calculated mobility is only 67% of the bulk mobility. This is due to larger phonon deformation potentials in a MOSFET than in a bulk material, which results from stress at gate dielectric and semiconductor interface [17].

The explanation of the mobility enhancement is described as follows. As a body thickness decreases, the energy difference between the first subband and second subband increases owing to quantum confinement effect, as shown in Fig. 3, where  $\Delta E$  is the energy difference between the first subband and second subband.

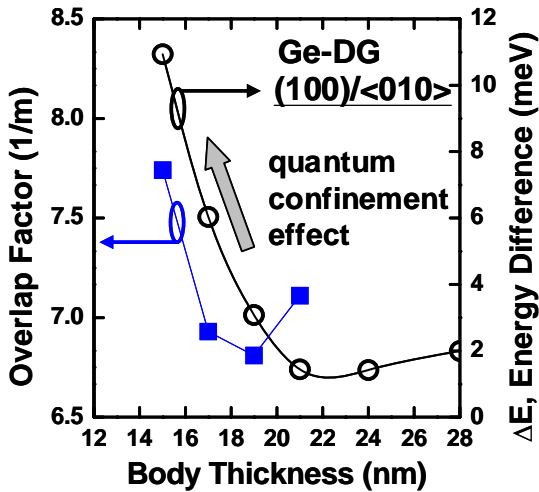


Fig. 3 The calculated overlap factor of the first subband and energy difference between the first subband and second subband in  $(100)/\langle 010 \rangle$  Ge-channel DG-pMOSFETs. An increase in both overlap factor and energy difference at a small body thickness is due to quantum confinement effect.

Therefore, larger energy difference leads to a reduction of intersubband scattering rate, and thus favors mobility improvement. However, when a smaller body thickness is considered, there is a wider distribution in momentum space due to the uncertainty principle. This can be understood from the illustration of Fig. 4.

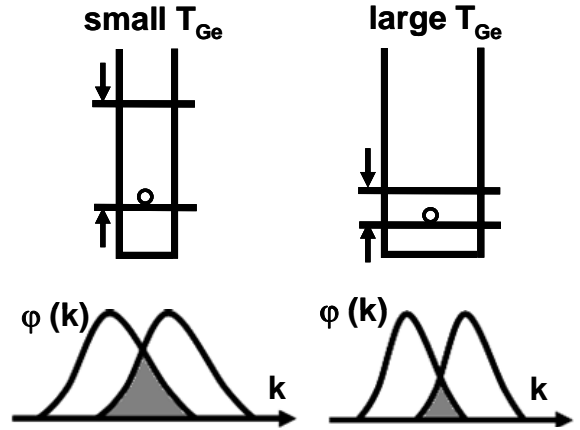


Fig. 4 Illustration of the overlap factor of an intrasubband scattering. The intrasubband scattering rate increases due to a larger overlap factor when a body thickness is reduced.

Only the shaded region contributes to the overlap factor. Thus, the spread of the wavefunction in momentum space results in a larger overlap factor and thus a larger intrasubband scattering rate. In this regime, the mobility accordingly decreases. As a consequence, there exists a window of a body thickness where the scattering rates can be minimized, giving rise to an onset of peak mobility.

#### IV. Summary

In summary, a two-dimensional Monte Carlo simulation is developed to explore the hole transport properties in a DG p-MOSFET. Our study indicates that the 2D hole mobility varies significantly with the geometry of the DG device. The hole mobility enhancement is about 40% for  $(100)/\langle 010 \rangle$  due to an optimization of the intrasubband and intersubband scattering rates.

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