Japanese Journal of Applied Physics
Vol. 43, No. 4B, 2004, pp. 1713–1716

Schottky Barrier Height Reduction and Drive Current Improvement in Metal Source/Drain MOSFET with Strained-Si Channel

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(Received September 18, 2003; accepted November 18, 2003; published April 27, 2004)

The use of strain to reduce contact resistance and improve the drive current of the Schottky barrier source/drain metal-oxide-semiconductor (MOS) transistor is proposed. The advantages of this approach were shown by theoretical calculation based on the non-equilibrium Green's function formalism. Furthermore, the interface dipole theory was firstly applied to the calculation in order to clarify the effects of strain and Fermi-level pinning on the Schottky barrier height. The calculated results indicate that bi-axial strain can reduce the Schottky-barrier height and increase complementary metal-oxide-semiconductor (CMOS) transistor drive current without disturbance of Fermi-level pinning, whereas hydrostatic strain has no effect on the barrier height because of the pinning. These results indicate the combination of the metal source/drain structure with a bi-axially strained Si channel can be beneficial for improving the drive current of nanoscale metal-oxide-semiconductor field-effect transistor (MOSFET). [DOI: 10.1143/JJAP.43.1713]

KEYWORDS: Schottky barrier height, metal source and drain, strained silicon, Green's function, Fermi level pinning, silicon band structure, interface dipole theory, charge neutrality level, deformation potential, hydrostatic strain, bi-axial strain

1. Introduction

Schottky barrier (metal) source/drain technology is promising for high-performance nanoscale metal oxide semiconductor field effect transistors (MOSFETs) because it provides shallow and low-resistivity source/drain regions with a simpler fabrication process and it can suppress the floating body effect of silicon on insulator (SOI) MOSFETs.[1–5] Furthermore, it should be noted that the hot carrier generated at the source barrier might increase the device speed of the ballistic MOS devices.[6] On the other hand, the primary challenge for this technology is reduction of the Schottky contact resistance (contact resistance between metal source/drain and Si-channel) in order to improve transistor drive current. It is known that the metal work function control is useful for reducing the contact resistance. For example, erbium silicide and platinum silicide can be used to reduce the Schottky barrier height E_b for NMOS and PMOS respectively. The typical values of E_b are 0.24–0.28 eV and 0.22 eV for the erbium silicide Schottky contact and the platinum silicide Schottky contact, respectively. Therefore, the contact resistance can be decreased by using these silicides. However, further barrier height reduction is difficult because of the Fermi level pinning effect.[1)]

In this paper, we propose the use of strain to reduce the Schottky barrier height and hence the contact resistance. As shown in Fig. 1, the energy levels of the 2-fold valley ($\Delta 2$) and 4-fold valley ($\Delta 4$) in the channel are affected by strain, so that the barrier height ($E_{b,\Delta 2}$) for the 2-fold valley can be significantly reduced whereas the barrier height ($E_{b,\Delta 4}$) for the 4-fold valley might be increased. The effects of strain and Fermi-level pinning on the Schottky barrier height are first presented, and then the advantages of using a strained-Si channel for the Schottky barrier source/drain MOSFET are described.

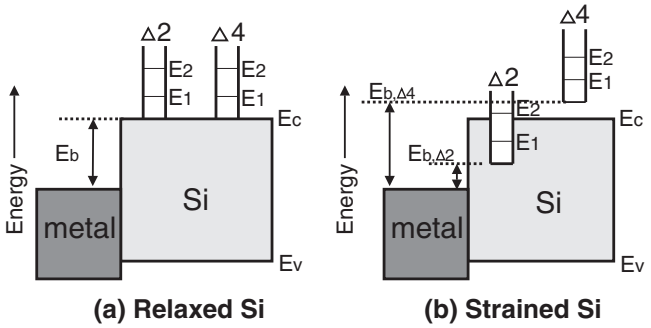

Fig. 1. Schematic diagram of energy band structure for the Schottky contact. (a) Relaxed Si, (b) Strained Si. $E_{b,\Delta 2}$: Schottky barrier height for the 2-fold valley, $E_{b,\Delta 4}$: Schottky barrier height for the 4-fold valley, E_1: the first sub-band level in 2-fold or 4-fold Valley, E_2: the second sub-band level in 2-fold or 4-fold Valley, E_C: conduction band, E_V: valence band, E_b: Schottky barrier height.

2. Simulation Model

For simplicity, a 12-nm (gate length) ballistic double-gate transistor structure was used for the device simulations (Fig. 2). The non-equilibrium Green's function method was used to include three carrier emission models at the Schottky contact, namely, the thermionic emission, the field emission and the thermionic field emission. (Fig. 3).[7)] Carrier effective masses (m_x, m_y, m_z) for each valley (for example, 2-fold valley, 4-fold valley, heavy hole band, etc.) and the strain dependence of the hole effective masses were included in the calculation.[8,9)]

In our simulation, one of the most important parameters is Schottky barrier height. The Schottky barrier heights for each valley were calculated by using the deformation potential parameters and the interface dipole theory to include the strain effect and the Fermi-level pinning effect on the barrier height (E_b).

2.1 Strain effect

In the case of the strained-Si channel formed on the

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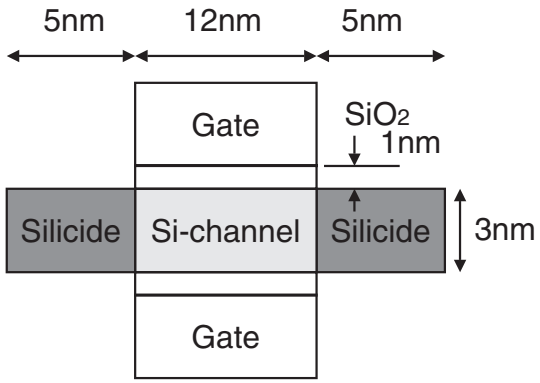

Fig. 2. Device structure used in the simulation: Ballistic double-gate MOSFET.

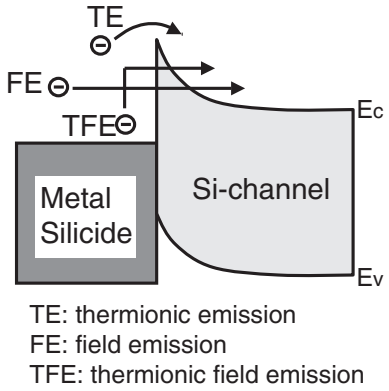

Fig. 3. Emission models included in the simulation. TE: thermionic emission, FE: field emission, TFE: thermionic field emission.

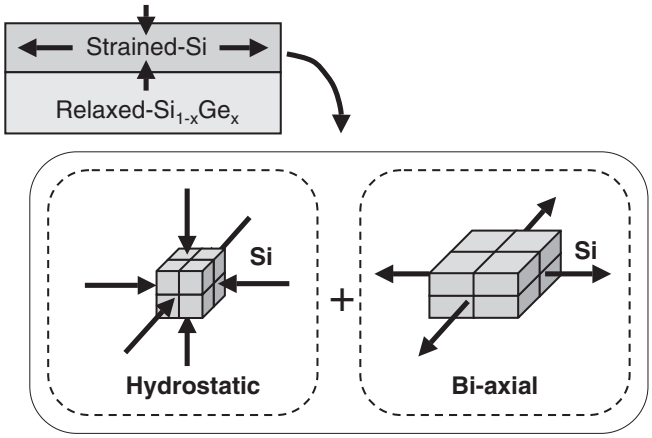

Fig. 4. Strain components in the strained silicon layer formed on the relaxed silicon germanium substrate. The strain is composed of the hydrostatic component and bi-axial component.

silicon germanium substrate, the strain is composed of the hydrostatic component and bi-axial strain component as shown in Fig. 4.

Figure 5 shows the valence- and conduction-band shifts caused by the stresses (composed of hydrostatic and bi-axial strain components). As shown in this figure, the hydrostatic strain lowers the energy levels of the conduction and valence bands, and the bi-axial strain splits the bands into valleys with different energy levels (2-fold, 4-fold, light hole(lh), heavy hole(hh) and split-off(so)).[9,10]

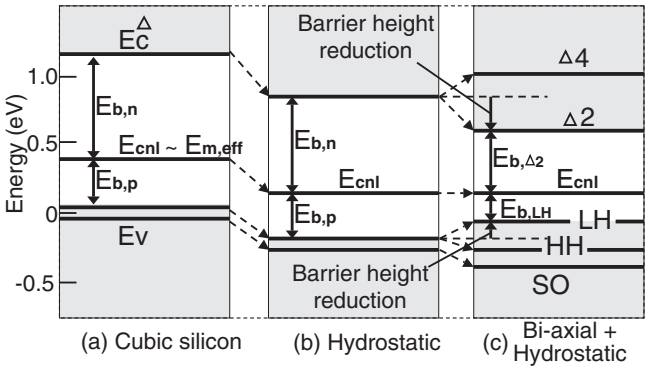

Fig. 5. Respective contributions of the hydrostatic and bi-axial strain components on the silicon valence and conduction bands for the strain situation experienced by a silicon layer on a relaxed silicon germanium substrate ($E_{xx} = E_{yy} = 0.02$, $E_{zz} = 0.016$). (a) Energy band for the cubic Si, (b) Energy band change caused by the hydrostatic strain component, (c) Energy band change caused by the bi-axial and the hydrostatic strain components. The charge neutrality level E_{cnl} and the Schottky barrier height E_b are also shown in the figure.

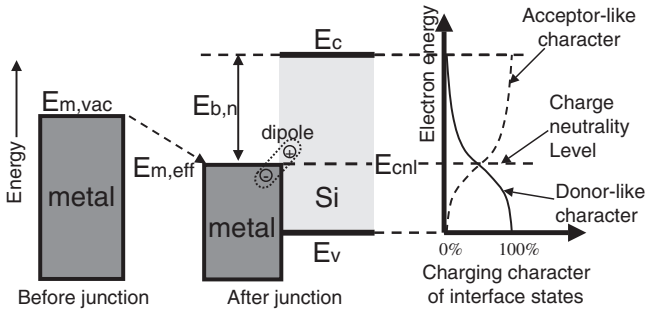

Fig. 6. Schematic diagram of the energy band structure of the Schottky contact and the electron energy dependence of the charging character of the interface states.

2.2 *Fermi level pinning effect*

According to the interface dipole theory, the metal work function is pinned near the charge neutrality level (E_{cnl})[11–13] (Fig. 6). The charge neutrality level is defined as the energy level at which the dominant character of the interface states changes from donor-like to acceptor-like. As shown in Fig. 6, the charge neutrality level is situated at around one-third of the band gap in the case of silicon. Therefore, the effective metal work function ($E_{m,eff}$) is different from the vacuum work function ($E_{m,vac}$) and can be calculated by using eq. (1) in Table I. The slope parameter S used in the equation was empirically found to be smaller than 0.1 in the case of silicon. Therefore, $E_{m,eff}$ is approximately equal to E_{cnl}. E_{cnl} can be calculated by using the cell averaged real space Green's function (eq. (2) in Table I) and silicon energy-band structure.[12,13] We calculated the silicon energy-band structure by using the empirical pseudo-potential method and included the strain effect in the calculation. Once E_{cnl} is calculated, $E_{m,eff}$ and E_b can be easily obtained.

3. Results and Discussion

3.1 *Charge neutrality level and Schottky barrier height*

Figure 5 shows the calculated E_{cnl} shift caused by the strain. It was found that hydrostatic strain changes E_{cnl}, but bi-axial strain has no effect on E_{cnl}. The reason for this result

Table I. Equations used for simulations.
$E_{m,eff}$: effective metal work function, $E_{m,vac}$: vacuum metal work function, E_{cnl}: charge neutrality level, S: slope parameter, Ψ_{nk}: wave function of Bloch wave vector k and band index n, E_{nk}: energy of the Bloch state, R: lattice vector, g: real space Green's function, G: cell averaged Green's function, G_c: Green's function for conduction band, G_v: Green's function for valence band.

Fermi level pinning:

$$E_{m,eff} = E_{cnl} + S \times (E_{m,vac} - E_{cnl}) \quad (1)$$

Real space Green's function:

$$g(r, r', E) = \sum_{nk} \frac{\psi^*_{nk}(r) \cdot \psi_{nk}(r')}{E - E_{nk}}$$

Cell-averaged real space Green's function:

$$G(R, E) \equiv \int dr \cdot g(r, r + R, E) = \sum_{nk} \frac{\exp(ik \cdot R)}{E - E_{nk}} \quad (2)$$

$$|G_C(R, E_{cnl})| = |G_V(R, E_{cnl})|$$

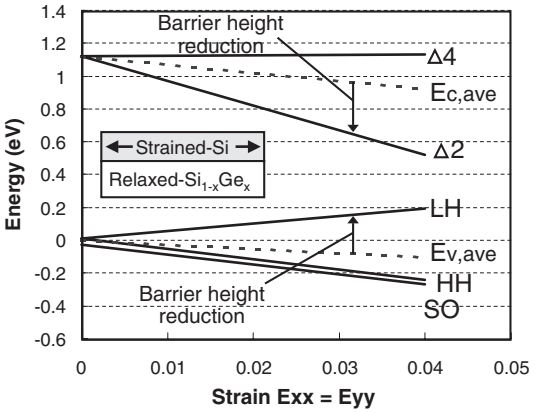

Fig. 7. Barrier height reduction caused by the strain (the hydrostatic strain and bi-axial strain) $E_{C,ave}$: average level of the conduction band, $E_{V,ave}$: average level of the valence band.

is that E_{cnl} is dependent only on the average level of the conduction band and valence band. It is known that the bi-axial strain splits the band into valleys with different energy levels, but it does not change the average band level. Therefore, E_{cnl} is dependent only on the hydrostatic component. Thus, the Schottky barrier heights for the 2-fold valley ($E_{b,\Delta 2}$) and the light hole valley ($E_{b,lh}$) can be reduced by bi-axial strain without the disturbance of Fermi-level pinning. On the other hand, hydrostatic strain is not useful for reducing E_b due to the Fermi-level pinning. Figure 7 shows the calculated E_b reduction caused by the strain.

3.2 Strain effects on the device characteristics

The effect of strain-induced E_b reduction on the performance of the ballistic double-gate MOSFET structure (Fig. 2) was studied next. Figure 8 shows the typical potential profile (for the first sub-band in the 2-fold valley) in the channel with and without the strain. As indicated in the Figure, E_b is reduced by $\sim$0.1 eV by 1% strain. This strain-induced barrier height reduction improves the drive current as shown in Fig. 9. Figure 9 shows the strain dependence of the drain current (I_d) and the threshold voltage (V_t) for complementary metal oxide semiconductor field effect transistors (CMOS-

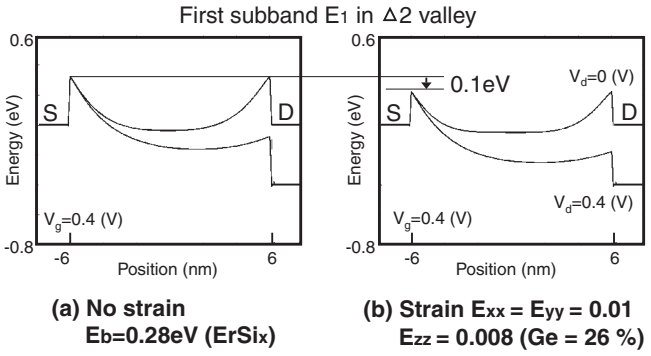

Fig. 8. Potential profile in the NMOS channel (first sub-band E_1 in 2-fold Valley). $V_g = 0.4$ V, $E_{c,ave} - E_{m,eff} = 0.28$ eV. (a) Relaxed Si, (b) Strained Si, $E_{xx} = 0.01$.

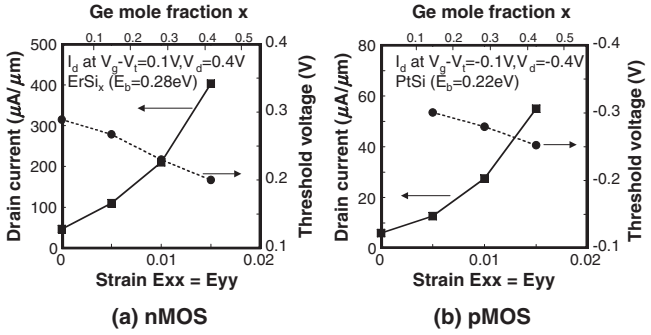

Fig. 9. Strain dependence of the drain current and the threshold voltage for (a) NMOS and (b) PMOS. (Calculation includes the Fermi-level pinning effect.)

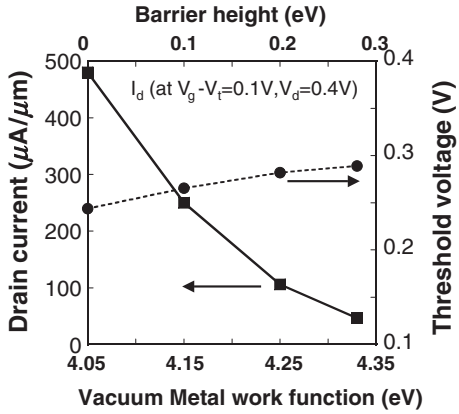

Fig. 10. Dependence of drain current and the threshold voltage on the barrier height (or metal work function). The barrier height is assumed to be adjustable by changing the metal (source) work function, without the pinning effect.

FETs). The exponential improvement in drain current with strain is attributable to the carrier mobility enhancement and the E_b reduction. And, it is noted that the threshold voltage decreases with the strain because of the barrier height reduction.

Next, the comparison between the strain effect and the metal work function effect on the NMOS drive current is presented. Figure 10 shows the dependence of I_d and V_t on the barrier height (or metal work function, assuming that E_b is determined by $E_{m,vac}$ without any pinning effect). From a comparison of Figs. 9(a) and 10, it can be seen that the drain

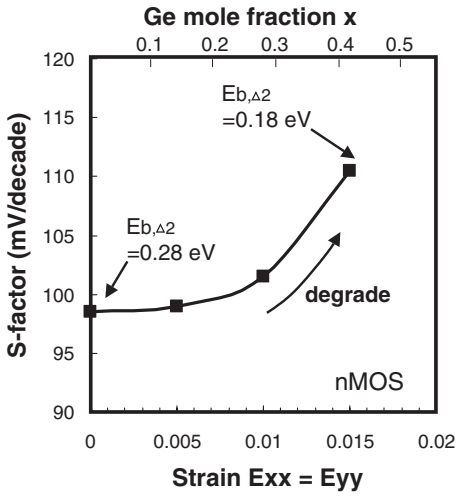

Fig. 11. Sub-threshold swing vs. strain characteristics (NMOS).

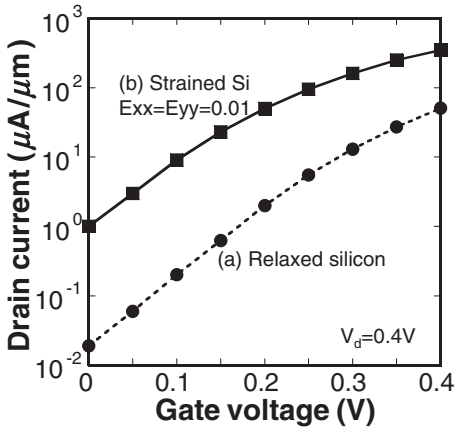

Fig. 12. Drain current vs. gate voltage characteristics (NMOS). (a) Relaxed Si, (b) Strained Si, $E_{xx} = E_{yy} = 0.01$.

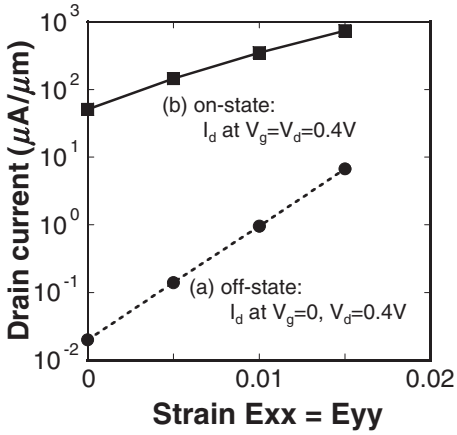

Fig. 13. Drain current vs. strain characteristics (NMOS). (a) off-state current, (b) on-state current.

current achieved with 0.015 strain is comparable to that which would be obtained for a device with the zero barrier height (metal work function of 4.05). It is known that the strain of 0.015 can be available by using the silicon germanium substrate technology. On the other hand, it is very difficult to form the zero barrier height Schottky contact because of the Fermi level pinning effect. Therefore, it is concluded that the bi-axial strain approach for improving drive current is more attractive than the metal work function engineering approach. It is a great advantage that the strain approach can reduce the Schottky barrier height without the disturbance of the Fermi level pinning effect.

However, it should be noted that the sub-threshold slope is degraded by the strain (Fig. 11), because the E_b reduction increases the off-state current as well as on-state current (Figs. 12 and 13). The reason for the sub-threshold swing degradation (off-current increase) is considered to be the short channel effect enhanced by the Schottky barrier height reduction. In order to improve the sub-threshold slope, a thinner Si-channel or thinner gate oxide can be used.

4. Conclusions

The use of strain to reduce contact resistance and improve the drive current of the Schottky barrier source/drain MOS transistor is proposed. The advantages of this approach were shown by theoretical calculation based on the non-equilibrium Green's function formalism. Furthermore, the interface dipole theory was firstly applied to the calculation in order to clarify the effects of strain and Fermi-level pinning on the Schottky barrier height. The calculated results indicate that bi-axial strain can reduce the Schottky-barrier height and increase CMOS transistor drive current without disturbance of Fermi-level pinning, whereas hydrostatic strain has no effect on the barrier height because of the pinning. These results indicate the combination of the metal source/drain structure with a bi-axially strained Si channel can be beneficial for improving the drive current of nanoscale MOSFETs.

Acknowledgements

We would like to thank Prof. Mark Lundstrom, Dr. Jing Guo, Dr. Yang-Kyu Choi, Mr. Daewon Ha, and Mr. Hideki Takeuchi for valuable discussions and support. We are also grateful to Dr. Kinya Usuda, Dr. Yoshitaka Tsunashima, and Dr. Kyoichi Suguro for their encouragement throughout this work. This research was partially supported under contracts MARCO/DARPA 2001-MT-887 and MDA972-01-1-0035.

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