Multiband Simulation of Uniaxially Stressed Silicon MOSFETs Based on Non-Equilibrium Green's Function Method

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1 Introduction

B-2-6

The strained silicon may be the noble alternative to the silicon in CMOS technology due to the improved transport characeristics [1]. We present the calculation of quantum electron transport in double-gate MOSFETs with uniaxially tensile strained silicon channel based on non-equilibirum Green's function (NEGF) [2] method considering the multiband structure of silicon [3]. The simulation results show that the presence of uniaxially strain induces the current enhancement in the devices.

2 Simulation Method

The calculation of quantum electron transport in strained channel MOSFETs is constructed based on nonequilibrium Green's function (NEGF) with the empirical tight binding approximation (TBA) model to obtain more realistic bandstructure. In the model, the system Hamiltonian is represented by a basis set of five atomic orbitals per atom $(s, p_x, p_y, p_z \text{ and } s^*)$ assuming nearest neighbour overlaps. The retarded Green's function may be obtained from the following equation

$$G^{R} = \left[(E - i0^{+})I - H - \Sigma_{L,R} \right]^{-1} (1)$$

where E is the energy and $\Sigma_{L,R}$ are the boundary selfenergies which take into account the effect of semi-infinite left and right contacts into the device. The device Hamiltonian, H, is a block tridiagonal matrix which contains the electrostatic potential, the orbital energies and the anion-cation matrix elements. By solving this Green's function, the local density of states and transmission function will be obtained. By summing these functions to the energy we can calculate the total carrier and current densities. In order to obtain self-consistent solution, the Green's function method and Poisson equation are iteratively performed.

The strained silicon bandstructure is obtained by using the empirical TBA model where the crystal lattice deformation is considered depending on the applied strain. In the TBA scheme, the strain effects can be included by adjusting the geometrical factors and the two-central integral parameters. The following Harrison's law is used to modify the two-center integral parameters.

$$H_{llm}^{s} = H_{llm} \left(\frac{\tau}{\tau^{s}}\right)^{\eta_{llm}} \tag{2}$$

where H_{llm}^s and H_{llm} are the two-center integral parameters with strain and without strain, respectively, and τ^s and τ are the distances between two atoms with strain and without strain. η_{llm} , which is orbital dependent, is the empirical parameters to describe how the two-center integral changes with the distance.

3 Results and Discussion

The device model under consideration is the double-gate (DG) MOSFETs with the carrier transport to be confined in [100] direction as shown in Fig. 1. The intrinsic channel is assumed to be silicon under uniaxial tensile strain where both source and drain are doped at $1 \ge 10^{20}$ cm⁻³, respectively. Six rotated ellipsoids of silicon conduction band which fold to two types of valleys, two- and four-fold valleys, are taken into the consideration.



Fig. 1. Schematic view of the nanoscale double-gate MOSFET under simulation. Six rotated ellipsoids of silicon conduction band are used.

Fig. 2 shows the drain current, I_{DS} , versus drain voltage, V_{DS} , characteristics of DG MOSFET with 6 nm channel length under 1%, 0.5% and 0% uniaxial tensile strain calculated at $V_{DS}=0.25$ V. We have found there is current enhancement with the presence of uniaxial tensile strain. The current enhancement is due to the increase in the sheet carrier density especially when the potential (first subband profile) at the source bottle neck point as demonstrated on Figs. 4 and 5. Although the first subband peak shifts upward with the tensile strain (Fig. 4), the conduction band minumum in the channel region moves downwards resulting in the increase of the sheet carrier concentration (Fig. 5) which gives consistent explanation of the current enhancement.

We also have varied the device channel length to see the effects of strain on the current enhancement as the channel length dependence. Fig. 5 shows the drain current characteristic of MOSFETs with 1% tensile strain for several channel length, $L_{ch} = 6, 8, 10, 12, 14$, and 16 nm. The on current with strain are compared with those of without strain in Fig. 6. The current enhancement is defined as the ratio of the current with strain with current without strain. The results show that the uniaxial tensile strain induces the current enhancement for all cases of channel length by a factor between 1.1 and 1.37. As the gate length becomes shorter, the enhancement factor is found to decrease monotonically since the device seriously suffers from short channel effects.

Acknowledgments

This study is financially supported by the Semiconductor Technology Academic Research Center (STARC).

References

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Fig. 2. Ballistic drain current (I_{DS}) vs drain voltage (V_{DS}) at $V_{GS} = 0.4$ V under 1%, 0.5% and 0% uniaxial tensile strain for <100> Si n-MOSFETs.



Fig. 3. Comparison of 1st subband profiles and carrier densities for <100> Si n-MOSFETs under with 1%, 0.5% and 0% uniaxial tensile strain calculated at $V_{DS} = 0.25$ V and $V_{GS} = 0.4$ V.



Fig. 4. The enlargement of fig. 3 at the source bottle neck or at the maximum of potential profiles.



Fig. 5. Ballistic drain current (IDS) vs gate voltage (VGS) for [100] Si n-MOSFETs with several channel length with 1% uniaxial tensile strain.



Fig. 6. Comparisons of on current with strain with those of without strain. The current enhancement is defined as the ratio of the current with strain with current without strain, calculated at $V_{DS} = 0.25$ V and $V_{GS} = 0.4$ V.