Mobility Calculation for Nanoscale Multi-Gate FETs with Arbitrary Two-Dimensional Cross Section with a Homogeneous Channel Including Strain Effects

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Abstract— **A mobility calculator for nanoscale multi-gate FETs with arbitrary two-dimensional (2D) cross section is described. It solves the coupled system of the 2D Schröedinger equation and the Poisson equation, therefore, the carrier quantization within the 2D cross section can be naturally considered. The strain effect is included by modifying the Hamiltonian. Both the conduction band and the valence band are implemented. The Kubo-Greenwood expression in the one-dimensional (1D) momentum space is used to calculate the mobility. Examples for a nanowire transistor and two FinFETs are presented. The interaction between the mobility calculator and the device simulator is described.**

Keywords-Mobility calculator;FinFET;Strain effect;

I. INTRODUCTION

For the next generations of the logic devices, the multi-gate FETs such as FinFETs and/or nanowire FETs will be introduced. Introduction of the non-conventional FETs brings two modeling issues for the inversion carrier mobility: Quantum confinement and strain effect.

First, for such devices, the enhanced control of the gate bias over the channel carrier is achieved by increasing the degree of the carrier confinement. For example, the FinFET has three surfaces surrounded by the gate. In contrast to the conventional MOSFET, the electronic structure of the inversion charge cannot be properly described as the 2D electron/hole gas. Its accurate description can be obtained from the solution of the 2D Schröedinger equation, instead of the 1D solution typically used for the conventional planar MOSFET.

Second, the mechanical stress inside the device has a critical importance in calculating the device performance. Changes in the bulk band structure due to the stress significantly change the important internal quantities like the inversion mobility.

Those two major issues from the mobility modeling perspective can be considered by the conventional device simulators only with partial success. In the case of quantum confinement, the conventional density-gradient (DG) simulation requires the additional, orientation-dependent, fitting parameter. Its values under the strained case are largely left as undetermined. Also no information about the subband structure can be obtained. Mobility models including the strain effects usually require extensive calibration for model parameters. In addition to such difficulties, another critical problem is the lack of predictability.

In order to address such modeling challenges, a mobility calculator for an arbitrary 2D cross section has been developed. It is based on the solution of the 2D Schröedinger equation, coupled with the Poisson equation. In this extended abstract, the scope of the work is briefly described and some selected results are presented. The interaction between the mobility calculator and the device simulator is also described.

II. MOBILITY CALCULATOR FOR ARBITRARY 2D CROSS SECTION

In this section, the overall structure of the mobility calculator is briefly described.

For a given cross section, the Schröedinger equation is solved in order to calculate the electronic structure of the inversion layer. Each eigenstate of the Schröedinger equation corresponds to a subband. By solving the 2D Schröedinger equation with the band model including the strain effect, two major modeling issues for the inversion carrier mobility in the multi-gate FETs, which are discussed in the Introduction, can be consistently taken care of.

Regarding to the mobility calculator, previous works are usually limited to either the 2D electron/hole gas [1][2] or the highly-symmetric 2D cross section [3]. Our mobility calculator can simulate the nanoscale multi-gate FETs with arbitrary 2D cross section.

The band model for electrons and holes is the ellipsoidal model and the 6-band k.p model, respectively. Strain effects are taken into account by considering the change of the mass due to the shear stress (electrons) or the Bir-Pirkus Hamiltonian (holes). Non-parabolicity is included for electrons [3]. The finite element method is employed to consider arbitrarily shaped cross section. Using the self-consistent solution with the Poisson equation, the mobility is calculated using the Kubo-

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Greenwood expression. Currently, the phonon scattering mechanisms are included in the mobility calculator. Implementation of other scattering mechanisms, including the surface-roughness scattering, is an on-going task. Model parameters for phonon scattering mechanisms can be found in [3] and references therein.

III. APPLICATIONS

In this section, some selected examples of the application of the mobility calculator are presented. A nanowire transistor and two bulk-type FinFETs (NMOS/PMOS) are considered. The interaction between the mobility calculator and the conventional device simulator is described at the end of this section.

A. Nanowire

Some benchmark tests are performed to validate the current implementation. The mobility in the nanowire with the diameter of 14nm is calculated. Electron density around Eeff~1MV/cm is shown in Fig. 1. Note that the electron density is not isotropic, due to the anisotropic masses of the three valleys in the conduction band.

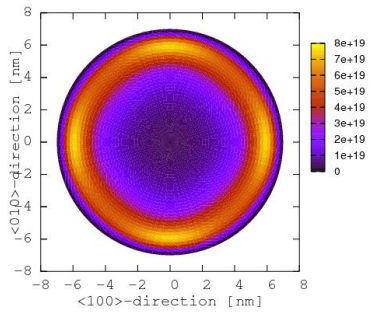

Figure 1. Electron density of a nanowire (with the diameter of 14nm) around Eeff~1MV/cm.

Fig. 2 shows the calculated mobility as a function of the effective field. Good agreement was obtained with the reference calculation in [3]. The effect of the non-parabolicity is shown in the figure. The subband energy measured from the local band edge, averaged with the square of the wave function, is identified as an effective kinetic energy. It is used for the non-parabolicity correction as in [3].

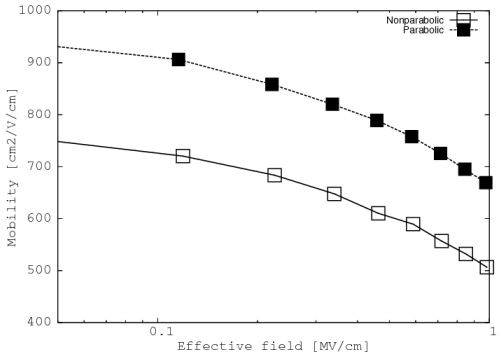

Figure 2. Phonon-limited mobility as a function of the effective field.

Fig. 3 shows the convergence behavior. The maximum change of the electrostatic potential is shown as a function of the Newton iteration number. The gate voltage is varied from 0.1V to 0.8V. The solution at the previous bias point is used as an initial guess without any correction. For strong inversion, it takes more iteration steps as observed in [4].

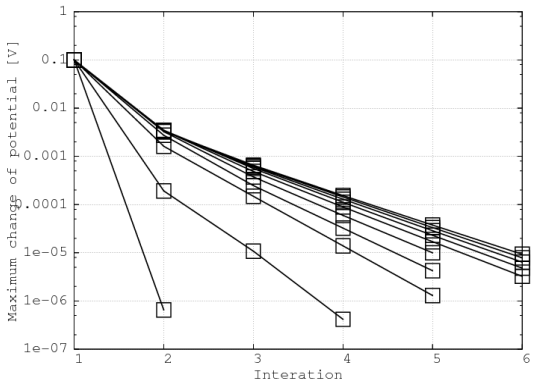

Figure 3. Convergence behavior of the nanowire simulation.

B. FinFET

The mobility calculator is applied to the simulation of the FinFET structures. Fig. 4 shows the cross section of the bulk-type FinFET considered in this work. Blue color in the figure represents the silicon fin region. The width of the fin is 10nm. It is surrounded by the square-shaped gate, which is red-colored in the figure. The conventional "(001)/<110>" configuration is adopted. Note that the mobility calculator can take into account of an arbitrary 2D cross section, although the FinFET considered in the example has an idealized shape.

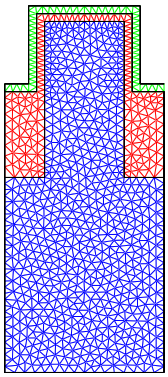

Figure 4. Cross section of the bulk-type FinFET structure. The width of the fin is 10nm. It is surrounded by the square-shaped gate (Green in the figure.)

Fig. 5 shows the inversion carrier density as a function of the applied gate voltage, under the relaxed condition. The carrier density is integrated over the entire fin. The gate workfunction for the N-FinFET and the P-FinFET is 4.3eV and 5.0eV, respectively.

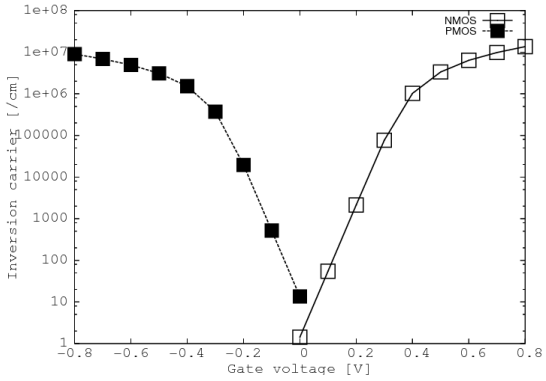

Figure 5. Inversion carrier density as a function of the applied gate voltage.

Fig. 6 shows the electron density in the fin at the gate voltage of 0.8V. The electron density shows its peak values around the upper corners. For rounded fins, the exact positions for peak values might be shifted.

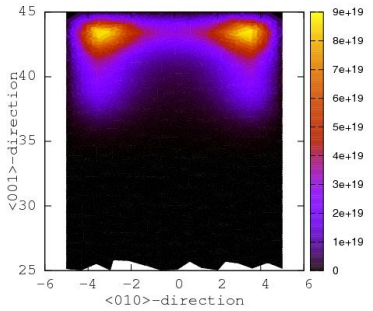

Figure 6. Electron density of the N-FinFET at Vg=0.8V. Axes in the figure represent the position in the device coordinates.

First, the N-FinFET results are shown. Fig. 7 shows the subband energies for the "(001)-valley". Typically, a few dozen subband energies per a valley in the conduction band are calculated for the mobility evaluation.

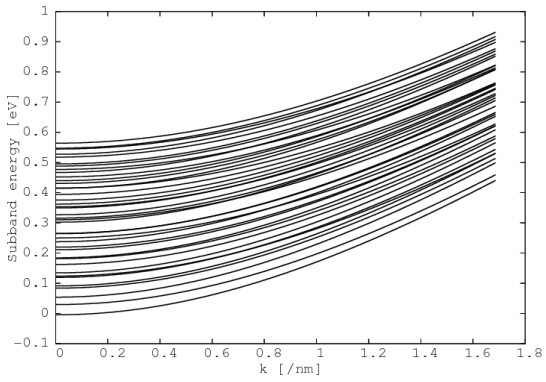

Figure 7. Subband energies of the N-FinFET at the gate voltage of 0.8V. First forty subband energies for the "(001)-valley" are shown.

Fig. 8 shows the calculated phonon-limited mobility of the N-FinFET as a function of the effective field. Again, the effective field is calculated by integrating the electric field over the fin cross section.

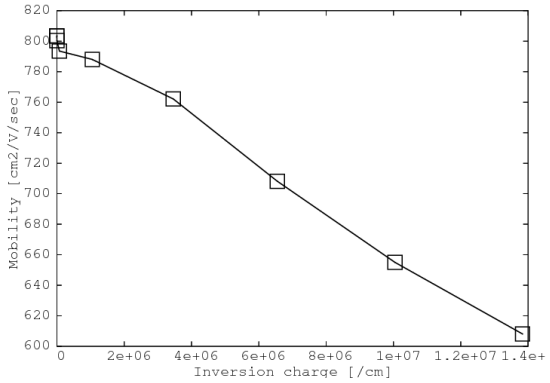

Figure 8. Phonon-limited mobility as a function of the inversion charge.

The mobility gain, defined as the ratio of the stress-enhanced mobility to the relaxed one, is calculated. Fig. 9 shows the mobility gain as a function of the applied stress. The positive value of the stress represents the tensile stress.

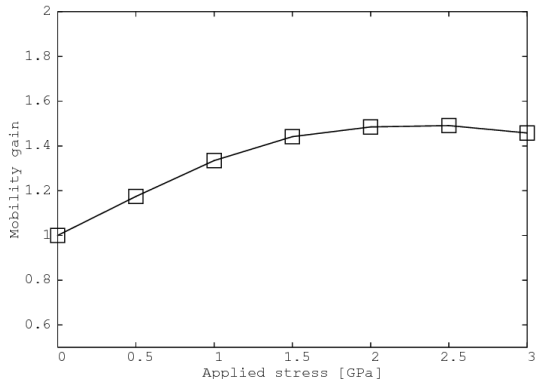

Figure 9. Mobility gain as a function of the applied stress at the gate voltage of 0V.

In the case of the P-FinFET, using the 6-band k.p model, the subband energies are shown in Fig. 10. The first 120 subband energies are shown. Note that many of them are degenerated.

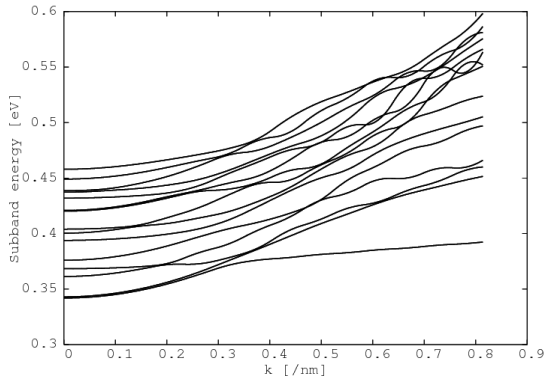

Figure 10. Subband energies of the P-FinFET at the gate voltage of 0V.

The mobility gain as a function of the applied stress for the P-FinFET is shown in Fig. 11.

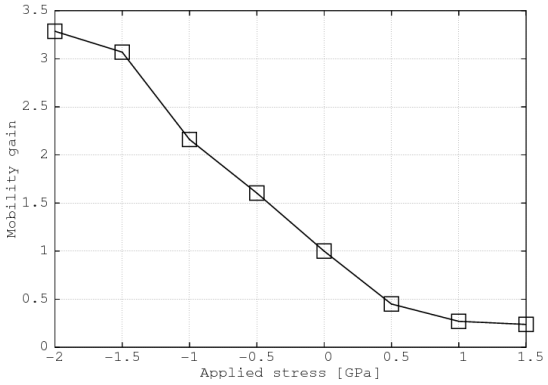

Figure 11. Mobility gain as a function of the applied stress at the gate voltage of 0V.

C. *Interaction with the device simulator*

When the mobility calculator imports the device structure used in the device simulator, realistic cross sections can be simulated without much effort. In order to enable the direct linkage between the mobility calculator and the device simulator, a routine for generating the cross section automatically from the given three-dimensional (3D) device structure is implemented.

Fig. 12 shows a set of 2D cross sections generated by slicing a typical 3D FinFET structure. Note that the original 3D FinFET structure can be readily used by a device simulator.

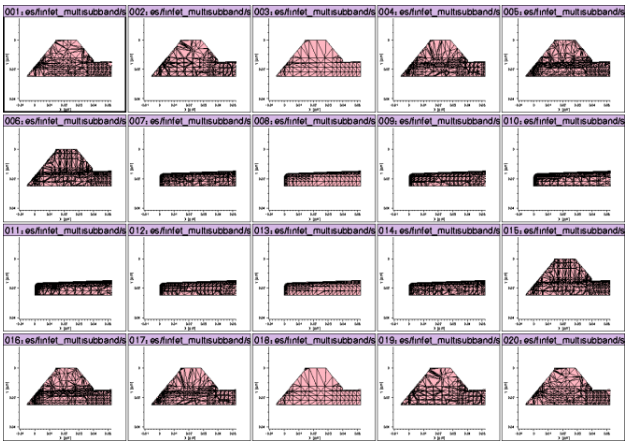

Figure 12. A set of 2D cross sections generated by slicing a typical 3D FinFET structure. Only silicon fins are shown in the figure.

The equilibrium electron density at the center of the channel is shown in Fig. 13. It is obtained by solving the Schröedinger-Poisson equations at the generated 2D cross section.

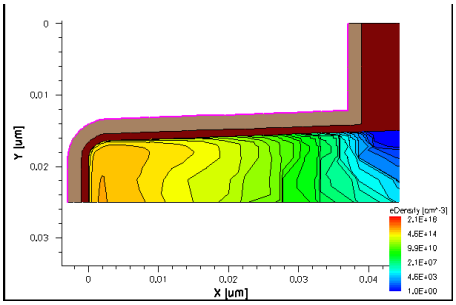

Figure 13. Equilibrium electron density at the center of the channel obtained by the mobility calculator.

Other results for more realistic cross sections directly obtained from the device structure will be presented elsewhere.

IV. CONCLUSION

The mobility calculator for the nanoscale multi-gate FETs is implemented. Both of the N-FinFET and the P-FinFET are simulated with strain effects. It is expected that the developed mobility calculator can be useful for exploring the optimal cross section of multi-gate FETs.

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