A Self-Consistent Simulation of InSb Double-Gate MOSFETs Using Full-Band Tight-Binding Approach

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Abstract

The electrostatics of InSb double-gate MOSFETs is simulated using a self-consistent solver which calculates channel bandstructure and carrier population by tight-binding (TB) approach. The Q-V_g characteristic and the Quantum Confinement Stark Effect (QCSE) are evaluated. By comparing with the results from the $k \cdot p$ method and effective mass approach, we show that full-band approach based on TB becomes more desirable when the channel is scaled down to a low dimensional quantum well. As the consequence of narrow channel width it is observed that the density of states (DOS) near band edges is decreased.

1 Introduction

InSb (Indium Antimonide) has been reported to have 50 times higher electron mobility than that of Si in the channel of MODFET [1]. However, the leakage current through the Schottky-contact in traditional MESFET or MODFET transistors of III-V compound semiconductor impedes the further scaling of such high-mobility devices. III-V MOSFET structure is thus desired and being actively pursued. In this paper, we simulate the electrostatics of InSb double-gate MOSFETs (shown in Fig. 1) with high-k gate dielectric (Al_2O_3) by applying a self-consistent tight-binding (TB) scheme. Through evaluating the Q-V_g characteristic and the Quantum Confinement Stark Effect (QCSE), we show that to model either the subthreshold or high gate-voltage electrostatics of InSb MOSFETs, the quantum confinement should be accurately accounted for. A self-consistent full-band approach is preferred.

2 Modeling and Simulation

We employ an $sp^3d^5s^*$ tight-binding (TB) model [2-3] to calculate the energy bandstructure of the 2D InSb ultra-thin-body (UTB). In the TB model, the wavefunctions in the channel are constructed as a linear combination of atomic orbitals (LCAO). Spurious energy states in the bandgap during calculation are eliminated by applying a hard-wall boundary condition at the interfaces between the channel and gate dielectrics. The external Hartree-Fock potential is incorporated into the diagonal entries of the Hamiltonian matrix for the channel.

To obtain a self-consistent solution, Schrödinger equation (i.e., the bandstructure calculation) is coupled with the 1D Poisson's equation, all in the direction perpendicular to the channel layer. The Hartree-Fock potential in the gate stack and

charge distribution in the channel are iterated until a self-consistent solution is obtained.

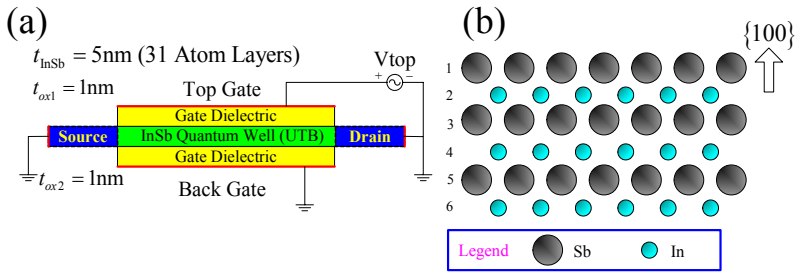

Figure 1: (a) The structure of InSb double-gate MOSFET. The channel is undoped and (100) oriented, with a high-k Al2O3 (Aluminum Oxide, $\varepsilon_{ox} = 9.6$) gate dielectric. To make our results comparable with other approaches, we adjust the gate-electrode work function such that when both gates are grounded, no potential drop exists and the sheet charge density in the channel is zero. (b) The In and Sb atom layers in the channel.

The solution of TB Schrödinger equation is rather time consuming. We used an adaptive mesh in the discretization of the Brillouin zone. Only those regions in the reciprocal space, which have eigen-energy around the Fermi level, are placed with dense mesh to improve computational efficiency. Bandstructure of the channel is calculated using a parallel computing platform. The Broyden update scheme [4] during Newton iteration is applied to improve the convergence behavior and to reduce the iteration times.

3 Results

The bandstructure calculated by TB is shown in Fig. 2. It can be observed that when the gate-voltage increases, the conduction band minimum drops faster than the valence band maximum, resulting in a *decreased* bandgap (from 0.44eV at $V_g = 0$ to 0.25eV at V_g = 1.4V). This is known as the Quantum Confinement Stark Effect (QCSE) and has been studied extensively for optical applications [5] but not in UTB-FETs in IC devices prior to this work based on the best of our knowledge. Although difference in bandgap reduction estimation by our TB approach requires experimental data to validate, our calculation shows that full-band self-consistent simulation is essential for modeling such effects.

It is observed that the bandgap of the channel (0.44eV) with 31 atom layers (5nm) is much bigger than that of the bulk (0.23eV), and it is caused by the quantum confinement (QC). It is also observed that the subband splitting resulting from the QC leads to a drop in the density of states (DOS) at the conduction band edge. This decrease of DOS tends to degrade the subthreshold behavior of the device, as the increase of the gate voltage induces fewer electrons in the channel. On the other hand, the subband splitting reduces inter-band scattering, and thus improves carrier mobility.

For applications requiring relatively high supply voltage, the conduction band minimum may drop below the Fermi level as shown in Figs. 2.b. The second conduction subband and the L valleys start to contribute to the electron population. The incorporation of L valleys changes the average electron effective mass in the channel, leading to the decrease of carrier mobility. This effect can only be modeled using a full band simulation, and extrapolation methods like $k \cdot p$ work less accurate than the TB approach.

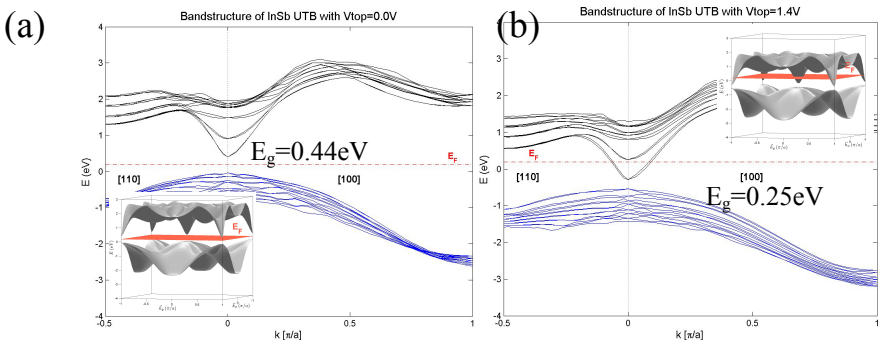

Figure 2: Bandstructure calculated using TB method for 5nm InSb channel. The bottom gate is grounded. Top gate voltage is (a) 0V and (b) 1.4V. The insets show the lowest conduction subband and highest valence subband in the Brillouin zone.

Figs. 3 illustrate the profile of potential drop and carrier distribution across the channel at the gate voltage of 0.4V. Fig. 4 shows further the sheet carrier density vs. top gate voltage calculated using TB, 8-band $k \cdot p$, and the effective mass approximation which is routinely used in device simulation software like Taurus [6]. While $k \cdot p$ has to be calibrated to generate correct sheet charge density, it is observed that effective mass approach tends to underestimate the sheet charge density after inversion. This is due to the overestimated bandgap as well as underestimated DOS calculated by the effective mass approximation, as has been pointed out by Rahman [7]. Table 1 shows the subthreshold slope calculated by all three approaches.

4 Conclusions

We implemented a self-consistent full-band tight-binding approach and an 8-band $k \cdot p$ approach to simulate the InSb MOSFETs with high-k dielectric. It is observed the atomistic level TB approach makes better estimation of electrical static characteristics than $k \cdot p$ and effective mass approaches.

Acknowledgements

Authors are indebted to various research grants from Chinese Government, including Project #: 9030-7016 (Computational Electronics) of NSFC and Project #: 2006CB302700 (Nano Scale Si Integrated Circuit Devices and Technology) of Ministry of Science & Technology. The support from parallel computing group in

Tsinghua National Laboratory for Information Science and Technology is greatly appreciated.

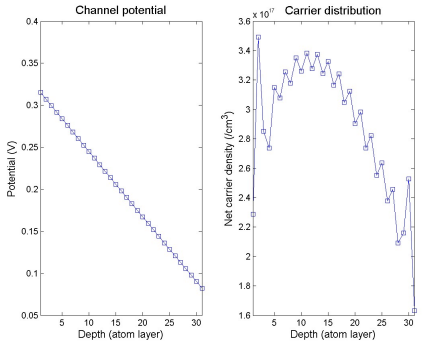

Figure 3: Electric potential inside the channel and carrier distribution among all 31 atom layers of InSb channel, calculated by the TB approach with top gate voltage of 0.4V. The serrated charge distribution is induced by the polar chemical bond between In and Sb atom layers.

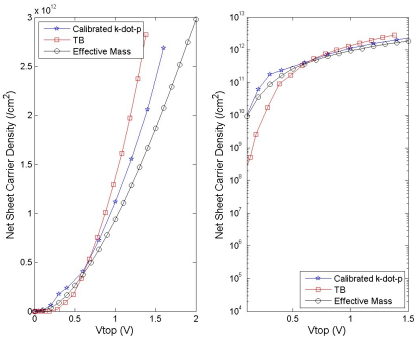

Figure 4: Comparison of $k \bullet p$, TB, and effective mass (EM) approach in calculating sheet charge density of InSb MOSFET.

	TB	Calibrated $k \bullet p$	Effective Mass	InSb MODFET [8]
Subthreshold slope (SS, mV/dec)	102.2	120.8	171.8	110

Table 1: Subthreshold slopes calculated by tight-binding, calibrated $k \bullet p$ and the effective mass methods.

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