2-D Self-Consistent Solution of Schrödinger Equation, Boltzmann Transport Equation, Poisson and Current-continuity Equation for MOSFET

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Abstract

We present a method of modeling quantum confinement effects in MOSFET's by solving the Schrödinger, Boltzmann, Poisson and current-continuity equations self-consistently.

1 Introduction

As MOSFET dimensions shrink into the nanometer regime, and oxide thicknesses reduce to the angstrom level, significant quantization effects occur in the motion of carriers perpendicular to the interface. We need to calculate the electronic properties of the quasi two-dimensional electron gas(2-DEG) and their effects on the MOSFET characteristics. Spinelli et al.(1998) presented a self-consistent two-dimensional drift-diffusion(DD) model for carrier quantization effects in the channel of highly-doped nMOSFET's. A quantum mechanical treatment of electron inversion layers of nMOSFET's is also incorporated in the hydrodynamic(HD) transport model by Wang et al.(1998). While these methods represent important contributions, they assume an equilibrium form at lattice or electron temperatures for the distribution function. However, it is well known that the channel distribution function is often far from equilibrium, which can lead to difficulties when populating the inversion layer subbands. Here we incorporate carrier quantization effects in the channel of highly-doped n-MOSFET's by solving the Schrödinger, Poisson, Boltzmann and Current-continuity equations self-consistently. The new method naturally accounts for highly nonequilibrium effects including velocity overshoot, and we populate the subbands according to the self-consistent nonequilibrium distribution function we obtain by solving the Boltzmann transport equation(BTE) (Liang et al. 1997).

2 Theory and realization

First we solve the Poisson equation, electron BTE and the hole current-continuity equation with the Spherical Harmonic Boltzmann(SHBTE) method. After getting self-consistent simulation results, we can solve the Schrödinger equation based on the potential energy $V(y)$ from the Poisson equation result. Using the new quantum-mechanical electron density, and a quantum mechanically updated form for the potential, we solve the Poisson equation, electron BTE and holes current-continuity equation again until these four equations converge. The flowchart of the QM-SHBTE is shown in Fig. 1. The complete model is given by:

$$\nabla_{\vec{r}}^2 \phi(\vec{r}) = \frac{q}{\epsilon_s} \left[n_q(\vec{r}) - p(\vec{r}) + N_A(\vec{r}) - N_D(\vec{r}) \right] \tag{1}$$

$$\frac{\partial f(\vec{r},\vec{k},t)}{\partial t} = -\frac{1}{\hbar}\nabla_{\vec{k}}\varepsilon \cdot \nabla_{\vec{r}} f(\vec{k},\vec{r},t) - \frac{q}{\hbar}\nabla_{\vec{r}}\phi(\vec{r},t) \cdot \nabla_{\vec{k}} f(\vec{k},\vec{r},t) - \left.\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}\right|_c \quad (2)$$

$$\frac{\partial p(\vec{r},t)}{\partial t} = \nabla_{\vec{r}} \cdot [\mu_p p(\vec{r},t)\nabla_{\vec{r}}\phi(\vec{r},t) + \mu_p V_t \nabla_{\vec{r}} p(\vec{r},t)] - R(n,p) \quad (3)$$

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dy^2}\psi_i(y) + V(y)\psi_i(y) = E_i\psi_i(y) \quad (4)$$

where $\phi(\vec{r},t)$ is potential, n_q is the quantum electron density, $f(\vec{r},\vec{k},t)$ is electron distribution function, $\left.\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}\right|_c$ is the collision term, $p(\vec{r},t)$ is hole concentration, m^* is effective mass along the direction perpendicular to the interface, $V(y)$ is the potential energy of the electrons, and E_i and ψ_i are the eigenenergy and eigenfunction of the ith subband respectively.

To solve the Schrödinger equation, we use a QL decomposition algorithm and a constant effective-mass approximation. After getting the energy levels and envelope functions, we populate the subbands and compute the electron density with the following

$$n_q(y) = \sum_i \mid \psi_i(y) \mid^2 \int_{E_i}^{\infty} f(E)D_i(E)dE \quad (5)$$

where $f(E)$ is the distribution function calculated directly by the Spherical Harmonic BTE solver, and $D_i(E)$ is the quasi 2-D density of states for electrons. Fig. 2 is the energy dispersion of a quantum well with subband energies. The integration of eqn.(5) corresponds to the area under distribution function curve between E_i and ∞ as shown in Fig. 3, which gives the electron concentration of each subband.

3 Results

Fig. 4 shows the classical and quantum electron concentration of the nMOSFET. The bias condition is $V_d = 0.05V$ and $V_g = 2.5V$. The subthreshold characteristics(log(I_d) vs. V_g) are shown in Fig. 5. We can see in this figure that the threshold voltage is increased by the quantization effect. Also the larger V_g is, the larger the difference between classical and QM results. We show I_d vs. V_g for high drain bias(V_d=1.0 V) in Fig. 6. As can be seen in this figure the difference between classical and QM result is reduced by increasing drain bias since DIBL will decrease the depth of the quantum potential well and pinchoff widens it. The I-V characteristics are shown in Fig. 7 and Fig. 8 for $L_g = 0.1\mu m$ and $L_g = 0.25\mu m$ respectively. They show that for these particular devices, the shorter the device length, the larger the difference between classical and QM results. Current density is shown in Fig. 9 and 10. We can see clearly the QM effect that the peak value of current density is several $\AA$ away from the SiO_2/Si interface, and the smooth current density usually implies a well-converged result.

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References

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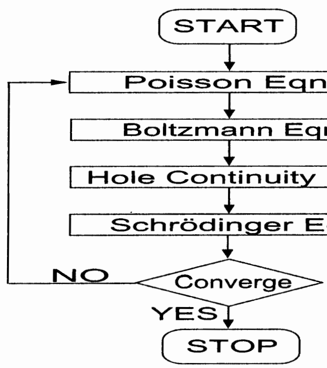

Fig. 1. The flowchart of the quantum BTE simulator

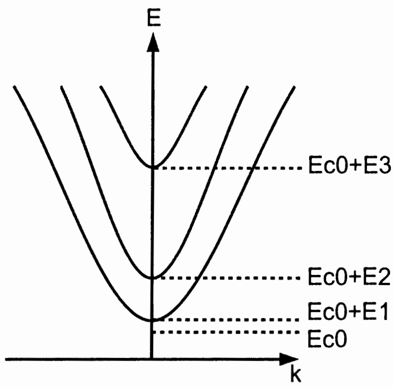

Fig. 2. Energy dispersion of quantum well.

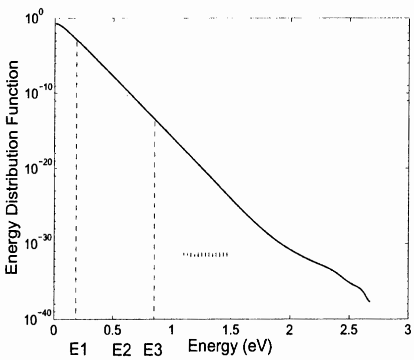

Fig. 3. The distribution function at surface for $V_g = 2.5V, V_d = 0.05V$.

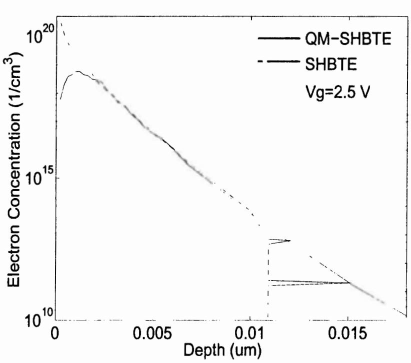

Fig.4. Electron density from surface to substrate at $V_g = 2.5V, V_d = 0.05V$.

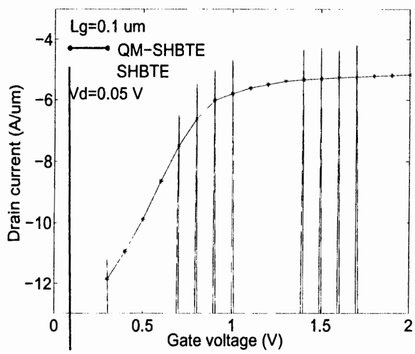

Fig.5. $\log(I_d)$ vs. V_g for $V_d = 0.05V, L_g = 0.1\mu m$.

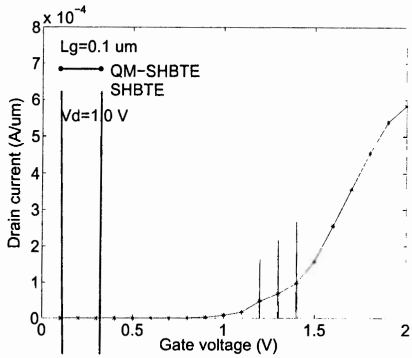

Fig.6. I_d vs. V_g for $V_d = 1.0V, L_g = 0.1\mu m$.

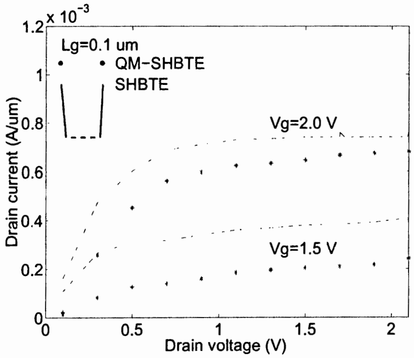

Fig.7. I-V characterictics for $L_g = 0.1\mu m$.

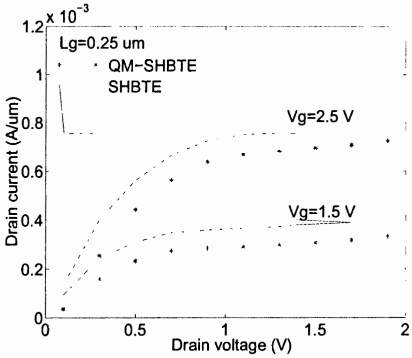

Fig.8. I-V characterictics for $L_g = 0.25\mu m$.

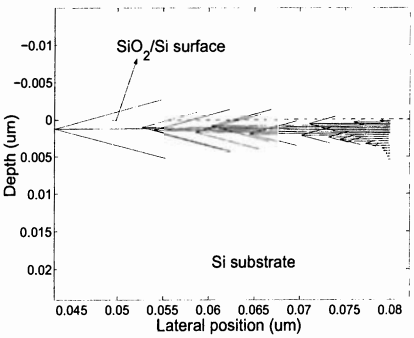

Fig.9. The current density maxium below surface of nMOSFET(QM-SHBTE).

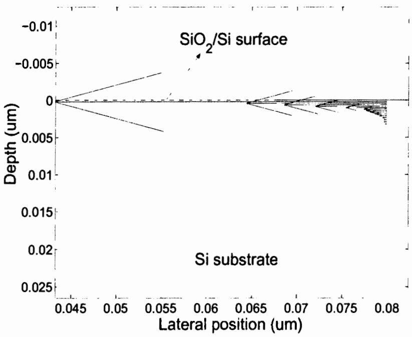

Fig.10. The current density maxium at surface of nMOSFET(SHBTE).