Monte Carlo Simulation of HEMT based on Self-Consistent Method

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Device simulation of HEMT (High Electron Mobility Transistor) has been carried out by ensemble Monte Carlo simulation, where two-dimensional motion of electrons confined in GaAs region at GaAs/AlGaAs heterointerface is taken into account. In order to develop a realistic device simulator of HEMT, we divide the channel region in meshes, and Schrödinger and Poisson equations are solved self-consistently to obtain electronic states of the two-dimensional electrons in a mesh. In addition the real space transfer from GaAs layer into AlGaAs barrier layer is taken into account.

INTRODUCTION

Device simulations of HEMT reported so far[1],[2] assume simplified models rather than reported here. Tomizawa *et al.*[1] divided the device into two-dimensional electron region and three-dimensional electron region by using a simplified relation without taking into account the energy of electrons at high fields. Ravaioli and Ferry[2] took into account two subband only. Zhou and Ferry[3] have recently reported numerical simulation of ultra-submicrometer HEMTs based upon a set of quantum moment equations.

Several authors reported the electron transport properties in GaAs/AlGaAs single heterostructures using Monte Carlo simulation[1],[2],[4]. The analysis is based on the electronphonon interaction model proposed by Price[5], where the quantized electrons (2DEG) are assumed to be scattered by bulk phonons and thus the wave functions calculated by the self-consistent analysis are used to evaluate the scattering rate. In our previous simulation of HEMT the

electric field parallel to channel is treated as uniform. In real device, however, the sheet electron density in the channel is not homogeneous and the electric field along the channel is not uniform, higher near the drain. In addition at high electric fields electrons are heated to form hot electrons which behave as three-dimensional electrons rather than 2DEG. Another important effect is the real space transfer of hot electrons between the GaAs layer and the AlGaAs barrier. Here we present Monte Carlo device simulator taking into account of non-uniform channel and real space transfer.

THEORETICAL MODELS

Calculation of Scattering Rate

We employ the self-consistent calculation method for estimating the subband structures of GaAs layer. In the energy band structure of GaAs, the lower conduction band minima are at Γ , L and X valleys. We calcu-

lated the eigen states of electrons in GaAs/AlGaAs hetero-junction assuming that the electrons in the three valleys are two-dimensional. In the case of GaAs/AlGaAs hetero-junction, we have to note that calculations should be carried out including electron transport in the spacer layer of AlGaAs because the barrier height between GaAs and AlGaAs is not so high to prevent the real space transfer. The electronic states of 2DEG in the Γ valley are calculated by solving the Schrödinger equation and Poisson equation self-consistently [6].

$$\left[-\frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} - e\phi(z) \right] \zeta_i(z) = E_i \zeta_i(z), \quad (1)$$

$$\frac{d^2\phi}{dz^2} = -\frac{1}{\kappa\epsilon_0} \left[\rho_{\text{depl}}(z) - e \sum_i N_i |\zeta_i(z)|^2 \right], \quad (2)$$

where m^* is the effective mass in Γ valley. $\phi(z)$ is the electrostatic potential, ρ_{depl} the charge density of the depletion layer, $\kappa\epsilon_0$ the static dielectric constant of GaAs, N_s the electron sheet density. Since the electrons in the interface of hetero-junction form two-dimensional states, Monte Carlo simulation requires the use of the scattering rate of the 2DEG interacting with three-dimensional phonons formulated by Price[5]. In our simulation, we take into account acoustic phonon, polar optical phonon, ionized impurity and inter valley phonon scatterings.

Device Simulation

In the previous 2DEG simulator the channel region is treated as uniform between the source and drain. In the real device, however, the channel region is not uniform. Another important factor for HEMT device simulation is to take into account the real space transfer from GaAs layer into AlGaAs barrier layer. In addition to these, electrons with high energy beyond the barrier height are not confined in the confinement potential but behave as three-dimensional electrons.

Figure 1 shows the device model used for the Monte Carlo simulation, where the channel length is $0.5 \mu\text{m}$ and the thickness of spacer layer of AlGaAs is $100 \text{ \AA}$. In order to simulate electron transport in non-uniform channel, we employed the following two

FIGURE 1 HEMT device structure used for the Monte Carlo simulation

steps. First, we evaluate the initial condition. We estimate the sheet electron density at each position between the source and drain using the current continuity relation along the channel. The drain current is estimated as

$$I_D = \frac{W}{L} \mu C [f(\phi_{sL}) - f(\phi_{s0})], \quad (3)$$

$$f(\phi_s) = \left(V_G + \frac{1}{\beta} \right) \phi_s - \frac{1}{2} \phi_s^2 - \frac{2}{3} a \phi_s^{3/2} + \frac{1}{\beta} a \sqrt{\phi_s} \quad \left(a = \frac{\sqrt{2\kappa\epsilon_0 q N_A}}{C} \right), \quad (4)$$

where W is the channel width, L the channel length, C the capacitance of AlGaAs layer and $\beta = q/k_B T = \mu/D$ (Einstein relation). ϕ_{s0} and ϕ_{sL} are surface potentials at the edge of source and drain. At the point of x measured from the source edge, the current is given by

$$I_D = \frac{W}{x} \mu C [f(\phi_s(x)) - f(\phi_{s0})], \quad (5)$$

where $\phi_s(x)$ is the surface potential at the point of x . Since the current is uniform along the channel, we can estimate $\phi_s(x)$ and $N_s(x)$.

Second, Monte Carlo simulation was carried out by evaluating the scattering rates of the electronic states in each mesh. Then two-dimensional Poisson equation was solved to obtain the potential distribution in the device. The Monte Carlo procedures were repeated until we obtain a steady state at an applied gate and drain voltages. We assume electrons are two-dimensional in the channel region from the source to

the pinch off point and three-dimensional beyond the pinch off point at the beginning of the simulation. At high electric fields, however, the two-dimensional electrons are heated to form hot electrons which are not confined in the region near the interface but behave as three-dimensional electrons. Therefore, an electron state in the channel region is defined as

$$\begin{cases} E_{\parallel} + E_i < E_{th} & \rightarrow 2D, \\ E_{\parallel} + E_i > E_{th} & \rightarrow 3D, \end{cases} \quad (6)$$

where E_i is the subband level and E_{th} the threshold energy. In the present simulation E_{th} is taken to be the conduction band discontinuity between GaAs layer and AlGaAs barrier layer at each valley. When the electronic state changes from two-dimensional to three-dimensional, we assume that the subband energy transfer to the kinetic energy in the z direction.

$$\frac{\hbar^2}{2m^*} k_z^2 = E_n \quad (7)$$

Also real space transfer from GaAs layer into AlGaAs barrier layer is treated in a similar fashion. When an electron changes from three-dimensional to two-dimensional, the electron is assumed to be confined in a subband E_i given by

$$E_i < \epsilon_z < E_{i+1}. \quad (8)$$

CALCULATION AND DISCUSSION

In the present simulation we take 20,000 electrons in the source and drain region, and the simulation carried out in the time scale up to 30 ps by 1 fs step.

Figures 2 and 3 show the electron distribution obtained by the present simulation, where the gate voltages are 0.5 V and 1.0 V, respectively, and drain voltage is 0.3 V. When the gate voltage is 0.5 V, there are few electrons transferred from GaAs layer into AlGaAs barrier layer. However, more electrons are transferred from GaAs layer to AlGaAs barrier layer when gate voltage is increased to 1.0 V. Figure 4 shows the electron drift velocity averaged in the meshes along z direction as a function of the position along the channel. When drain voltage is low, the drift velocity between the source and the drain increases in

FIGURE 2 Electron distribution obtained by the Monte Carlo simulation in the HEMT for gate voltage 0.5 V and drain voltage 0.3 V

FIGURE 3 Electron distribution obtained by the Monte Carlo simulation in the HEMT for gate voltage 1.0 V and drain voltage 0.3 V

FIGURE 4 Average electron drift velocity in the channel region is plotted as a function of position for gate voltage 0.5 V

proportion to the field parallel to the surface. As the drain voltage becomes high, the velocity saturation is observed near the drain region.

Figure 5 shows I_D versus V_D characteristics estimated from the present simulation. Although experimental results are not available for comparison, the present results show a reasonable feature of I_D versus V_D characteristics of a HEMT.

FIGURE 5 I_D versus V_D characteristics of the HEMT obtained by the Monte Carlo simulation

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