Two-Dimensional Static Numerical Modeling and Simulation of AlGaN/GaN HEMT*

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Abstract: AlGaN/GaN HEMTs are investigated by numerical simulation from the self-consistent solution of Schrödinger-Poisson-hydrodynamic (HD) systems. The influences of polarization charge and quantum effects are considered in this model. Then the two-dimensional conduction band and electron distribution, electron temperature characteristics, I_d versus V_d and I_d versus V_g, transfer characteristics and transconductance curves are obtained. Corresponding analysis and discussion based on the simulation results are subsequently given.

Key words: AlGaN/GaN HEMT; 2D modeling and simulation; polarization charges; quantum effects
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1 Introduction

In recent years, $Al_xGa_{1-x}N$/GaN high electron mobility transistors (HEMTs) have received considerable attention due to their advantages and potential in materials and devices. With the rapid progress of material growth and the maturing of lithography and other related device fabrication technologies, many exciting experimental results have been reported[1~3]. An obvious trend is that gate length and device dimensions are becoming shorter, which is necessary for higher frequency operation. On the other hand, as an effective tool for device design, computer aided design technology faces severe challenges for heterostructures. These have caused modeling and simulation to lag behind[4,5].

$Al_xGa_{1-x}N$/GaN HEMT modeling has many new features, such as spontaneous and piezoelectric polarization, quantization effects, and hot-electron and non-local transport. Therefore, a simulator with more complex physical models and a higher level of numerical robustness is required. Although the commercial simulators have made progress in solving these difficulties, newly introduced material characteristics, device structures, and physical effects are still open issues that limit their usage[6~8]. In this paper, a new two-dimensional (2D) small $Al_xGa_{1-x}N$/GaN HEMT model is proposed, and corresponding simulation results are shown.

2 2D AlGaN/GaN HEMT model

The structure and simulation mesh information are shown in Fig. 1.

2.1 Basic equations

The finite-difference method (FDM) is a conventional numerical way to solve the Schrödinger-Poisson-transport equations. Since the size quantum effect is only in the direction of the hetero-interface, Schrödinger's equation is given by

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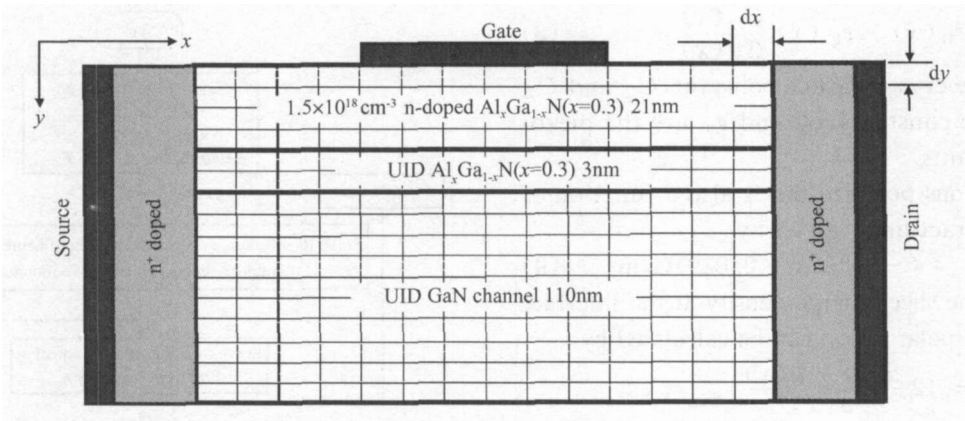

Fig. 1 Device and simulation mesh structure $L_{sd} = 500\text{nm}$, $L_g = 100\text{nm}$

$$-\frac{\hbar^2}{2}\times\frac{d}{dy}\left(\frac{1}{m^*(y)}\times\frac{d}{dy}\right)\psi_k(y) + V_x(y)\psi_k(y) = E_k\psi_k(y) \quad (1)$$

where E_k is the eigenenergy, ψ_k is the corresponding envelope function for subband k, V is the potential energy, $\hbar$ is Planck's constant divided by 2π, and m^* is the effective mass.

The 2D Poisson equation has the form:

$$\nabla\cdot[\varepsilon_s(y)\nabla\phi(x,y)] = -\frac{q}{\varepsilon_0}[N_D(x,y) - n(x,y)] \quad (2)$$

where ε_s is the position dependent dielectric constant, ϕ is the electrostatic potential, N_D is the ionized donor concentration, and n is the electron density distribution.

In a quantum well with an arbitrary potential energy profile, the potential energy V is related to the electrostatic potential ϕ as follows:

$$V_x(y) = -q\phi_x(y) + \Delta E_c(y) \quad (3)$$

where ΔE_c is the conductance band offset.

The drift-drain (DD) and hydrodynamic (HD) models are derived from Boltzmann's transport equation (BTE). They are extremely important in the classical transport field. It has been shown that the HD model describes the carriers' movement more accurately, especially for non-local effects, electron velocity overshoot, and high field effects[9,10]. Because of the compact confinement of the 2DEG in the y direction, only the electron transport in the x direction is considered. The HD model is then

$$\frac{1}{q}\nabla\cdot J_n = -U \quad (4)$$

$$\nabla\cdot S_n = E\cdot J_n - Uw_n - n\frac{w_n - w_0}{\tau_{wn}} \quad (5)$$

The auxiliary equations for current density flux and electron energy flux are

$$J_n = -q\mu_n n(x)\nabla\left(\phi(x) - \frac{k_B T_n(x)}{q}\right) + qD_n\nabla_n(x) \quad (6)$$

$$S_n = -k_n\nabla T_n(x) - (w_n + k_B T_n(x))\frac{J_n}{q} \quad (7)$$

Equation (4) is the electron continuity equation, where U denotes the generation-recombination rate. Equation (5) is the energy balance equation (EBE), in which the last term represents the energy loss rates of the electrons by scattering in the relaxation time approximation. Here w_n, w_0 are the average electron energy and equilibrium energy, respectively. Here we neglect the kinetic energy in view of numerical iteration convergence, so $w_n \approx \frac{3}{2}k_B T_n$ (the convention in commercial simulators). We use the constant relaxation time 0.4ps. The current density is given by Eq. (6), where μ_n and D_n are the electron mobility and the diffusion coefficient. D_n and μ_n satisfy the Einstein relation. The mobility model adopts the high field correlated model[11] with $\mu_0 = 800\text{cm}^2/(\text{V}\cdot\text{s})$, $v_{sat} = 1\times10^7\text{cm/s}$. Equation (7) gives the electron energy flux, where k_n is the thermal diffusion coefficient. S_n comprises the thermal conductive term and the energy convective term.

2.2 Polarization effects and interface model

There are both linear and nonlinear models for the computation of polarization charge, and it is still not certain which is more suitable[12,13]. In this paper the linear model is chosen for its physically conceptual simplicity.

The strain-induced piezoelectric polarization is expressed by

$$P_{PE}(Al_xGa_{1-x}N) = 2\frac{a(0) - a(x)}{a(x)}\times$$

$$[\, e_{31}(x) - e_{33}(x)\frac{C_{13}(x)}{C_{33}(x)}\,] \qquad (8)$$

where a is the crystal lattice constant, C_{13} and C_{33} are the elastic constants, e_{31} and e_{33} are the piezoelectric constants.

Spontaneous polarization is also a function of the Al mole fraction x, given by

$$P_{sp}(x) = (-0.052x - 0.029)\ \mathrm{C/m^2} \qquad (9)$$

Finally, the sheet charge density at the interface induced by the polarization can be calculated by

$$|\sigma(x)| = \left| 2\frac{a(0)-a(x)}{a(x)}\left\{ e_{31}(x) - e_{33}(x)\frac{C_{13}(x)}{C_{33}(x)}\right\} + P_{sp}(x) - P_{sp}(0)\right| \qquad (10)$$

For the AlGaN/GaN hetero-structure, consideration of the discontinuity of ε and the polarization sheet charge at the interface is necessary, as shown below:

$$E_{AlGaN}\varepsilon_{AlGaN} - E_{GaN}\varepsilon_{GaN} = -\sigma \qquad (11)$$

3 Numerical method and self-consistent solution

Equations listed in the section above show that the Poisson equation is 2D, but the effective mass equation and the carrier transport equation are both one-dimensional (1D), parallel and normal to the channel direction respectively. Figure 2 shows schematically the conversion of the 2D problem into two 1D ones. It is necessary to convert the 2D electron surface density to a 3D body distribution. The flow chart in Fig. 3 illustrates the 2D solution procedure.

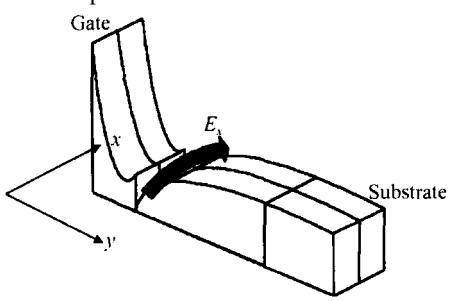

Fig. 2 Sketch of converting 2D problem into two 1D ones

For an arbitrary node [i, j], the linearized finite difference form of Poisson's equation is

$$\frac{dx}{dy}\phi_{i-1,j} + \frac{dy}{dx}\phi_{i,j-1} + \frac{dy}{dx}\phi_{i,j+1} + \frac{dx}{dy}\phi_{i+1,j} - 2\left(\frac{dx}{dy}+\frac{dy}{dx}\right)\phi_{i,j} = -\frac{dxdy}{\varepsilon}q(N_D - n)_{i,j}dx \qquad (12)$$

For the nodes at the interface, it is transformed into:

$$\frac{dx}{dy}\varepsilon_{AlGaN}\phi_{i-1,j} + \frac{dy}{2dx}(\varepsilon_{AlGaN}+\varepsilon_{GaN})\phi_{i,j-1} + \frac{dy}{2dx}(\varepsilon_{AlGaN}+\varepsilon_{GaN})\phi_{i,j+1} + \frac{dx}{dy}\varepsilon_{GaN}\phi_{i+1,j} - \left(\frac{dx}{dy}+\frac{dy}{dx}\right)(\varepsilon_{AlGaN}+\varepsilon_{GaN})\phi_{i,j} = -dxdyq(N_D - n)_{i,j} - \sigma_{i,j}dx \qquad (13)$$

where dx and dy are mesh spacings in the x and y directions. Typically, dy is chosen to be smaller than dx in order to obtain a finer grid in the device channel for accurate simulations.

Here the current flux equation is discretized in the same way as in the existing discretization scheme for the HD model where the conventional S-G scheme is adopted[10]. The discretized form of the HD model is

$$J_n = qD_n\frac{\Delta T}{\Delta x \lg(\frac{T_{i+1}}{T_i})}\times[B(\Delta)\frac{n_{i+1}}{T_{i+1}} - B(\Delta)\frac{n_i}{T_i}] \qquad (14)$$

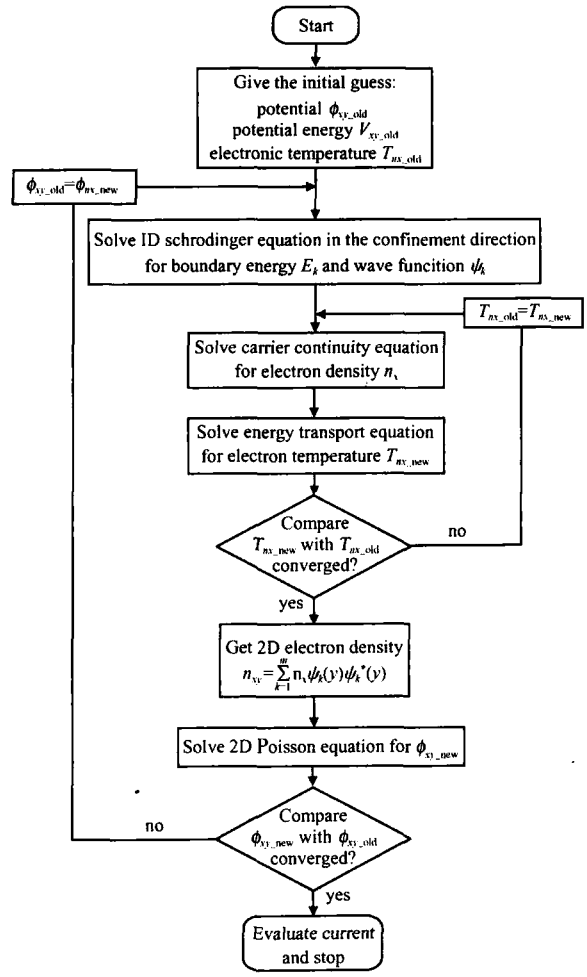

Fig. 3 Flow chart illustrating the solution procedure

where $\tilde{\Delta} = \frac{\lg(T_{i+1}/T_i)}{\Delta T}[\frac{q}{k_B}\Delta\phi - 2\Delta T]$ and $B(\cdot)$ is the Bernoulli function.

The discretized form of the energy flux equation for electrons is

$$S_n = -(\frac{5}{2} + c_n)\frac{k_B D_n}{\Delta x}\tilde{N}[B(\tilde{\Phi})T_{i+1} - B(-\tilde{\Phi})T_i] \quad (15)$$

where

$$\tilde{N} = \frac{\Delta T}{\lg(\frac{T_{i+1}}{T_i})} \times \frac{n_{i+1}}{T_{i+1}} \times \frac{B(\tilde{\Delta})}{B(\tilde{\Phi})} \quad (16)$$

$$\tilde{\Phi} = \frac{\lg(\frac{T_{i+1}}{T_i})}{\Delta T}(\frac{q}{k_B}\Delta\phi - \Delta T) - \lg\frac{n_{i+1}}{n_i} \quad (17)$$

$$\tilde{\Phi} = \frac{\frac{5}{2}}{\frac{5}{2} + c_n}\tilde{\Phi}$$

4 Results and discussion

Figures 4 and 5 show the simulated electron distribution and conduction band obtained from the 2D Schrödinger-Poisson-transport solver. The spontaneous and piezoelectric polarization charges are included, which are implemented in the direction normal to the AlGaN/GaN HEMT interface. The intentional doping density in the AlGaN barrier layer is $1.5\times10^{18}\,cm^{-3}$, and the background carrier concentration at room temperature is about $1\times10^{16}\,cm^{-3}$. The density of the 2DEG is $1.58\times10^{13}\,cm^{-2}$ at $V_g = -1V$.

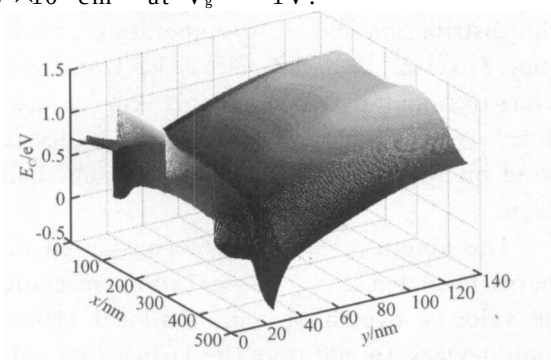

Fig. 4 2D conduction band $V_g = -1V$, $V_{sd} = 1V$

From Fig. 4 we can see that the conduction band energy varies with V_{ds} in the direction along the channel. Normal to the channel, as electrons are transferred from the doped AlGaN layer to the undoped channel layer, the potential barrier is formed in the doped region near the interface,

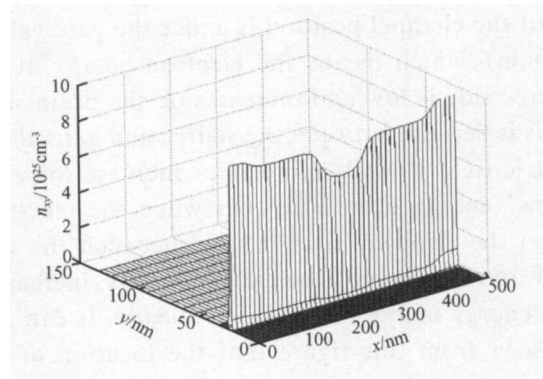

Fig. 5 2D electron distribution $V_g = -1V$, $V_{sd} = 1V$

and a potential well is located in the channel layer. Because of the conduction discontinuity of the hetero-structure, the electrons are located near the interface. But since they are affected by the size quantum effect, they are not exactly at the interface but penetrate into the barrier layer. The peak of the electron concentration in the potential well is close to the hetero-interface, as can be seen in Fig. 5.

In our simulation, the kinetic energy is not specified, so the temperature term is the only parameter representing the electron energy. On the basis of the meaning of electron temperature, the following simulation results can be easily understood.

Figure 6 shows the electron temperature at every channel position with different V_d. The electron temperature, namely the electron energy, ascends with the increasing V_d. This suggests that the enhancement of V_d increases the electric field in the channel, which accelerates the electrons and increases their energy.

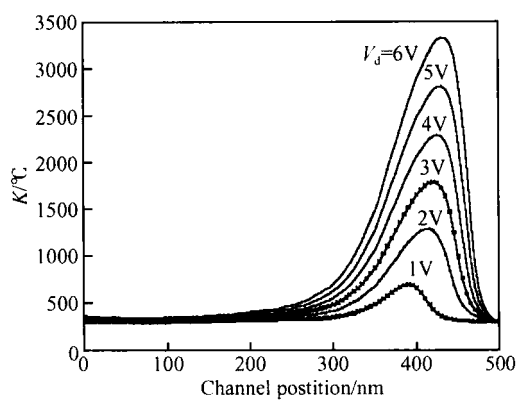

Fig. 6 Electron temperature in the channel $V_g = -1V$

Another observation from Fig. 6 is that the electron temperature does not change noticeably

until the channel position is under the gate (about 200nm), which means the electron energy at the source side is low and increases on the drain side. This is because between the source and gate, the electric field is weak and cannot increase the electrons' energy effectively, but when the electrons enter the stronger electric field between the gate and drain, they are accelerated quickly, increasing the energy of the electrons drastically. It can also be seen from this figure that the location of the maximum electron temperature value is closer to the drain side because of the electron velocity overshoot.

Figure 7 shows the curves of electron temperature peak value versus V_d at different gate voltages. From this figure we can see that the electron temperature changes more quickly at high V_g than at low V_g.

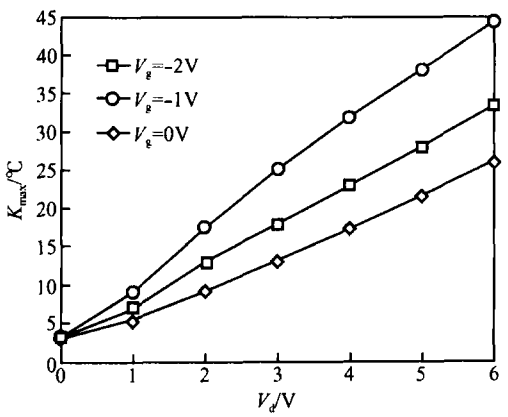

Fig. 7 Electron temperature peak value

The typical DC output and transfer characteristics of the AlGaN/GaN HEMT are shown in Figs. 8 and 9, respectively. The maximum saturation current is 1522mA/mm when $V_g = 0$V. Equation (6) in the HD model mentioned above shows that the total current comprises a diffusion term because of the carrier density gradient, a drift term under the electric field and thermal flux from the 'hot' area to the 'cold' area. The threshold voltage is about -6.5V, and the maximum transconductance is 262mS/mm.

5 Conclusion and future work

In this paper, a 2D simulation of a AlGaN/GaN HEMT is carried out by self-consistently solving the Poisson-Schrödinger-HD equations while

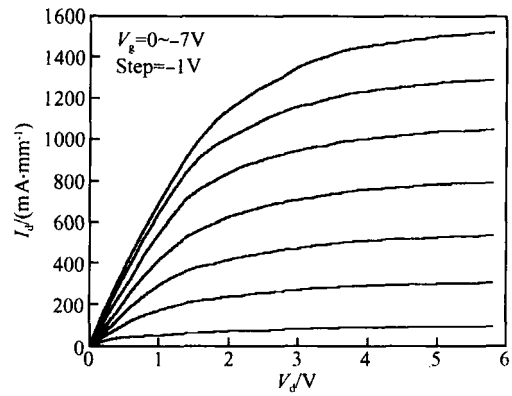

Fig. 8 DC output characteristics of AlGaN/GaN HEMT

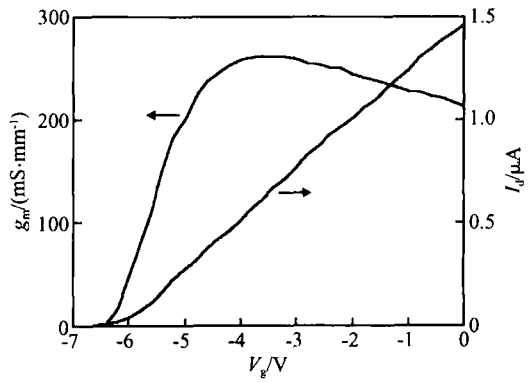

Fig. 9 DC transfer characteristics of AlGaN/GaN HEMT

taking into account the spontaneous and piezoelectric polarization effects necessary in GaN-based devices, from which the conduction band and electron distribution, electron temperature characteristics, I_d versus V_d and I_d versus V_g, transfer characteristics, and transconductance curves are obtained. Corresponding analysis and discussion based on the simulation results are subsequently given.

The kinetic energy is not considered in the energy term, but it plays a vital role, especially for the velocity overshoot and non-local effects in small devices. In addition, the lattice thermal diffusion equation is also helpful for obtaining more accurate results. As for the numerical methods, a rectangle is rougher than a triangular mesh. Finally, working out the complicated arithmetic is another requisite to ensure computational efficiency and steady convergence. Further study is therefore necessary.

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AlGaN/GaN HEMT 二维静态模型与模拟*

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摘要: 考虑 AlGaN/GaN 材料的自发、压电极化效应和量子效应,通过泊松方程、薛定谔方程和流体力学方程组的数值自洽求解方法,对 AlGaN/GaN HEMT 的二维静态模型与模拟问题进行了研究,得到了器件区域的导带图、二维电子气分布、电子温度特性、直流输出和转移特性,并对模拟结果进行了分析与讨论.

关键词: AlGaN/GaN 高电子迁移率晶体管; 二维模型与模拟; 极化电荷; 量子效应

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