Influence of a two-dimensional electron gas on current–voltage characteristics of $Al_{0.3}Ga_{0.7}$ N/GaN high electron mobility transistors*

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The J–V characteristics of $Al_tGa_{1-t}N$/GaN high electron mobility transistors (HEMTs) are investigated and simulated using the self-consistent solution of the Schrödinger and Poisson equations for a two-dimensional electron gas (2DEG) in a triangular potential well with the Al mole fraction $t = 0.3$ as an example. Using a simple analytical model, the electronic drift velocity in a 2DEG channel is obtained. It is found that the current density through the 2DEG channel is on the order of 10^{13} A/m^2 within a very narrow region (about 5 nm). For a current density of 7×10^{13} A/m^2 passing through the 2DEG channel with a 2DEG density of above 1.2×10^{17} m^{-2} under a drain voltage $V_{ds} = 1.5$ V at room temperature, the barrier thickness L_b should be more than 10 nm and the gate bias must be higher than 2 V.

Keywords: two-dimensional electron gas, high electron mobility transistor, heterointerface, nitride semiconductor

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1. Introduction

GaN-based transistors exhibit excellent high frequency, high power, and high temperature performances and have the potential to replace Si- and GaAs-based transistors for a number of applications[1−5] due to the outstanding electronic properties of $Al_tGa_{1-t}N$/GaN heterostructure, such as a high saturation velocity and a high breakdown voltage.[6,7] In $Al_tGa_{1-t}N$/GaN heterostructure, there exist strong piezoelectric and spontaneous polarization fields due to different lattice constants between the $Al_tGa_{1-t}N$ and GaN layers, and both polarizations can induce a high sheet charge density on the order of 10^{13}/cm^2[8,9] located in the heterointerface. Electrons tend to compensate the high positive polarization sheet charge, so that in the region of the barrier close to the $Al_tGa_{1-t}N$/GaN heterointerface a large number of electrons will have accumulated to shape a triangular potential well in the GaN layer.[10] These electrons accumulated in the potential well will form a two-dimensional electron gas (2DEG) channel and lead to a high current density through the channel. Some experimental and theoretical studies of transport properties for $Al_tGa_{1-t}N$/GaN heterostructure have been reported in the last decade.[11−15] However, up to now, most studies about the relationship between current and voltage have been restricted only to classical models,[16−18] which cannot reflect the wave properties of an electron in 2DEG. In the present paper, we use the self-consistent method to study a high electron mobility transistor based on $Al_tGa_{1-t}N$/GaN heterostructure with the Al mole fraction $t = 0.3$ as an example. The envelope wave function of electrons in 2DEG can be derived from the self-consistent solution of Schrödinger and Poisson equations in the finite triangle-shaped quantum well. However, the envelope wave function of the electrons is only considered to be inefficient in order to derive the relationship between current and drain voltage. Here we adopt an approximate drift-velocity model to incorporate the scattering process of electrons,[16,18] thereby being able to describe the characteristics of the current and drain voltage easily.

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2. Model and method

For the 2DEG in the $Al_tGa_{1-t}N$/GaN heterostructure, the motions of electrons are restricted in the direction normal to the interface between the two materials (z direction) only, while they are free in the x and the y directions. Hence we can separate the Schrödinger equation into space components in different directions in rectangular coordinates, so the x- and y-coordinate dependence of the wave function, which can be derived from the solution of Schrödinger equation, can be separated from the z-coordinate dependence, resulting in a plane-wave solution for the motion of the electrons in the x–y plane.[19] Therefore, the wave function corresponding to the α-th subband level can be expressed as

$$\psi_\alpha(x,y,z) = \frac{1}{S_{xy}} \mathrm{e}^{\mathrm{i}(k_x x + k_y y)} \psi_\alpha(z), \tag{1}$$

in which S_{xy} is the area of sample, k_x and k_y represent the wave vectors in the x–y plane, and ψ_α is the envelope wave function.

The probability current density responding to the α-th subband level can be written as

$$j_{y\alpha} = \frac{1}{S_{xy}} \frac{\hbar k_y}{m^*} |\psi_\alpha(z)|^2, \tag{2}$$

where $\hbar$ is the reduced Planck constant and m^* is the effective electron mass. Then the current density can be expressed by the following equation

$$J_y(z) = e \frac{\hbar k_y}{m^*} \sum_\alpha n_\alpha |\psi_\alpha(z)|^2, \tag{3}$$

in which e is the electron charge, n_α is the 2DEG density in the α-th subband level and can be expressed as

$$n_\alpha = \frac{m^* k_\mathrm{B} T}{\pi \hbar^2} \ln\left(1 + \exp\left(\frac{E_\mathrm{F} - E_\alpha}{k_\mathrm{B} T}\right)\right), \tag{4}$$

with k_B being the Boltzmann constant, T the temperature, E_F the Fermi energy, and E_α is the α-th subband level.

Due to the fact that the current density depends on the 2DEG density in the channel, it is necessary to find factors that may influence the value of the 2DEG density. We adopt a model from which we can find the relationship between the 2DEG density and the gate bias.

The electric field in the AlGaN barrier can be expressed as follows:[20]

$$F_\mathrm{b} = -\frac{e(\sigma - n_\mathrm{s})}{\varepsilon_0 \varepsilon_\mathrm{r}} = -\frac{e(V_\mathrm{b} - V_\mathrm{g}) + E_\mathrm{F} - \Delta E_\mathrm{C}}{e L_\mathrm{b}}, \tag{5}$$

where ε_0 is the vacuum dielectric constant and ε_r is the relative dielectric constant, σ is the polarization sheet charge density at the $Al_tGa_{1-t}N$/GaN heteojunction, n_s is the 2DEG density in the well, eV_b is the surface barrier height, ΔE_C is the conduction band offset between the barrier materials, and L_b is the barrier thickness. The parameters in Eq. (5) can be obtained from Refs. [7] and [20].

For relative dielectric constant $\varepsilon_\mathrm{r}(t) = -0.5t + 9.5$, surface barrier height $eV_\mathrm{b} = 3$ eV, conduction band offset $\Delta E_\mathrm{C} = 0.7[E_\mathrm{g}(t) - E_\mathrm{g}(0)]$, and the band gap $E_\mathrm{g}(t) = [6.13t + 3.42(1-t) - t(1-t)]$ eV, where t is Al mole fraction, so the band gap of the $Al_tGa_{1-t}N$/GaN structure, of which the smallness can result in bad confinement of the polarization induced sheet carrier density, increases linearly with t increasing.[19] Moreover, the limitation of the mobility of the 2DEG, which is caused by the high lattice and the thermal mismatch between the $Al_tGa_{1-t}N$ layer and the GaN layer which can result in a high density of structural defects in $Al_tGa_{1-t}N$ and rough interface, increases rapidly with t increasing, hence $t < 0.15$ and $t > 0.4$ have not been applicable to high-quality transistors to date.[7] In the present paper, we take $t = 0.3$ as an example, as the characteristics of the $Al_tGa_{1-t}N$/GaN heterostructures with different t values ranging from 0.15 to 0.4 are similar.

The polarization induced sheet charge density can be obtained from the following formula:[7]

$$|\sigma(t)| = \Big|2\frac{a(0) - a(t)}{a(t)}\Big[e_{31}(t) - e_{33}(t)\frac{c_{13}(t)}{c_{33}(t)} + P_\mathrm{sp}(t) - P_\mathrm{sp}(0)\Big]\Big|, \tag{6}$$

where lattice constant $a(t) = (-0.0077t + 0.3189)$ nm, elastic constants $c_{13}(t) = (5t + 103)$ GPa, and $c_{33}(t) = (-32t + 405)$ Gpa, piezoelectric constants $e_{31}(t) = (-0.11t - 0.49)$ C/m^2 and $e_{33}(t) = (0.73t + 0.73)$ C/m^2, spontaneous polarization $P_\mathrm{sp}(t) = (-0.052t - 0.029)$ C/m^2.

ψ_α, E_α, and E_F in the above equations can be derived from the self-consistent solution of the Schrödinger and Poisson equations, the procedure can be described as follows.

Considering the effective mass approximation, the Schrödinger equation can be written as

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left(\frac{1}{m^*}\frac{\partial \psi(z)}{\partial z}\right) + V(z)\psi(z) = E\psi(z), \tag{7}$$

where $V(z)$ is the interaction potential of electrons and can be written as

$$V(z) = \Delta E_\mathrm{C}(z) + V_\mathrm{H}(z) + V_\mathrm{ex}(z). \tag{8}$$

Here, V_H is the Hatree potential of the electrostatic

interaction which is induced by charges in the system, and $V_{\rm ex}$ is the exchange–correlation potential of charges which can be given by Lundqvist's formula[21]

$$V_{\rm ex} = -\Big[1 + 0.7735\chi \ln\Big(1 + \frac{1}{\chi}\Big)\Big]\frac{e^2}{21\pi\alpha\chi},$$
$$\chi = r_{\rm s}/21, \quad r_{\rm s}^{-1} = \Big[\frac{4\pi}{3}n(z)\Big]^{1/3} a_{\rm B},$$
$$\alpha = \Big(\frac{4}{9\pi}\Big)^{1/3} a_{\rm B}, \tag{9}$$

where $a_{\rm B}$ is the Bohr radius, $n(z)$ is the density of electrons which can be written as

$$n(z) = \sum_{\alpha} n_\alpha |\psi_\alpha(z)|^2, \tag{10}$$

and $V_{\rm H}$ obeys the Poisson equation

$$\frac{\rm d}{{\rm d}z}\Big[\varepsilon(z)\frac{\rm d}{{\rm d}z}V_{\rm H}(z)\Big] = e^2\rho(z),$$
$$\rho(z) = \sum_i \sigma_i \delta(z - z_i) + N_{\rm D}^+(z) - n(z), \tag{11}$$

where σ_i is the surface density of polarization charges at the i-th interface, $n(z)$ and $N_{\rm D}^+$ are the density of electrons, and the density of ionized donors, respectively.

From the neutrality condition, we have the following formula:

$$\int_0^L \Big[\sum_i \sigma_i \delta(z - z_i) + N_{\rm D}^+(z) - n(z)\Big]{\rm d}z = 0, \tag{12}$$

where L is the width of the two materials on the growth direction.

It is difficult for us to know the characteristics of the current and the drain voltage if we consider only the wave functions in the 2DEG, it is necessary to know the effect of the transferred-electrons. Therefore, in this paper, we use an approximate analytic formula to represent the electron drift velocity, which includes variety of electronic scattering processes, and it is given by[18]

$$\upsilon_y = \frac{\hbar k_y}{m^*} = \frac{\mu_0 F_y + \upsilon_{\rm s}\big(F_y/F_{\rm C}\big)^\beta}{1 + \big(F_y/F_{\rm C}\big)^\beta} \tag{13}$$

where μ_0 is the low-field mobility, $\upsilon_{\rm s}$ is the saturation velocity, $F_{\rm C}$ is the electrical field corresponding to the peak velocity, and F_y is the electric field through the channel which can be estimated as $F_y = V_{\rm ds}/L_{\rm ds}$, in which $V_{\rm ds}$ is the drain voltage and $L_{\rm ds}$ is the length of the channel. $\beta = 4$ is the best found to fit the data that are provided by the Monte-Carlo simulation,[18,22] so it is adopted in this paper.

3. Results and discussion

A typical $Al_tGa_{1-t}N/GaN$ heterostructure with $t = 0.3$ is depicted in Fig. 1. It shows the two lowest subband energy levels and the corresponding envelope wave functions in the triangle-shaped quantum well. The self-consistent potential and the normalized wave functions including the polarization effect for the two lowest energy levels are also shown in Fig. 1. From this figure, one can see that the electrons in the ground subband energy level are accumulated in the area near the interface of the two materials and the Fermi energy level is between the two lowest subband energy levels, thus it is easy for us to estimate that there are about 90 percent electrons in the lowest subband energy level, which means that the properties of the HEMT are determined mainly by electrons in the lowest subband. In addition, the quantum well is triangle-shaped at the heterointerface, which is a result of the large number of charges induced by piezoelectric and spontaneous polarization fields. It is worthwhile pointing out that because of the electron accumulation at the heterointerface, the electronic properties in the 2DEG have a significant influence on the transport characteristics of the high electron mobility transistor (HEMT). Therefore, by carefully controlling electron transport in the 2DEG, it is possible to design the desirable HEMT devices.

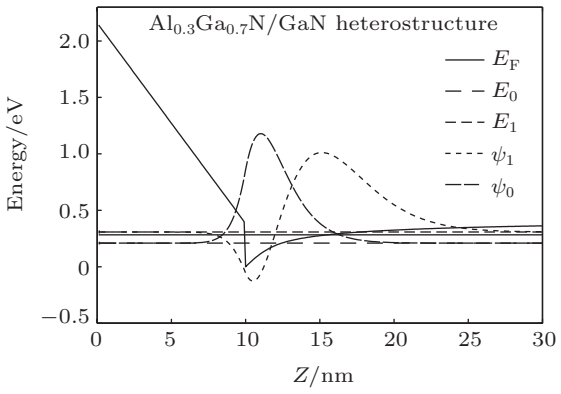


Fig. 1. Fermi energy, the two lowest energy subbands, and the corresponding wave functions in the two-dimensional electron gas (2DEG) channel, with Al mole fractions t being 0.3.

Results for the density $n_{\rm s}$ of the 2DEG versus the gate bias $V_{\rm g}$ with barrier thicknesses of 9 nm, 10 nm, and 11 nm, which can sufficiently reflect the fact that the thicker barrier induces a higher density of the 2DEG clearly, are shown in Fig. 2. It is indicated that the density of the 2DEG increases as the gate bias increases, and they have a linear relationship.

From Eq. (5), we can understand the relationship easily. For a given $eV_b = 3$ eV, the $Al_tGa_{1-t}N$ barrier thickness L_b is related to the 2DEG density as shown in Fig. 2. For different values of barrier thickness L_b, the different slopes indicate the different capacitive abilities of the 2DEGs. As the barrier thickness L_b increases further, the density of the 2DEG reaches a critical value. At the same time, a large number of electrons accumulated in the 2DEG channel cause a strong screen effect at the heterointerface and reduce the responsive ability to the gate bias V_g. In general, it is known that the depletion state and the saturation state will occur for the 2DEG channel when the applied voltage exceeds a critical value.[23] For the gate bias, a low voltage is selected within the voltage range, i.e., the extreme gate bias is not considered here. In this case, however, the insulation layer and the 2DEG channel can be considered as an electric capacitor, and as gate bias increases, the charge at the surface of the electric capacitor increases correspondingly. In fact, a balance of the total charges needs to be kept in the material, there are a lot of electrons to compensate positive charges, and subsequently the electrons are accumulated in the triangular potential well at the heterointerface. As a result, the density of the 2DEG increases as the gate bias increases.

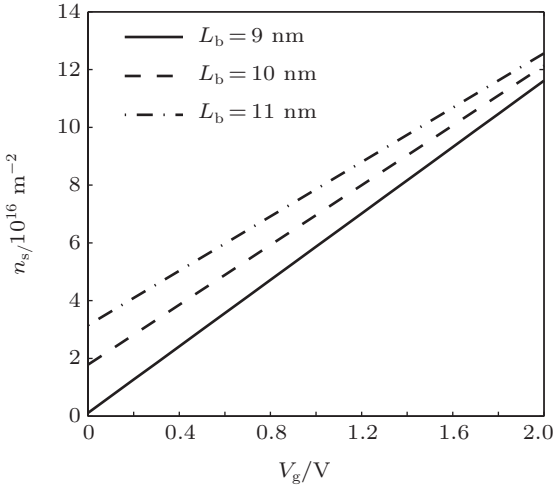


Fig. 2. Plots of the 2DEG density versus the gate bias with barrier thicknesses of 9 nm, 10 nm, and 11 nm.

As is well known, when the drain voltage increases, the electric field increases correspondingly, and so does the drift velocity which has a significant influence on the properties of J–V of the $Al_{0.3}Ga_{0.7}N$/GaN high electron mobility transistor. However, the drift velocity cannot increase infinitely. There will be a saturation region of the drift velocity of electrons, as a result of which, the current, which most depends on the drift velocity of electrons in the channel, has a saturation area when the drain voltage increases. The characteristics of current density against drain voltage under gate biases of 0 V, 1 V, and 2 V, which can sufficiently indicate that a higher gate bias will result in a higher current density, are shown in Fig. 3, from which we can easily recognize the saturation value of the current densities under different gate biases. We know that electrons have a lot of probabilities of scattering and other effects that can resist the drift of electrons with increasing drift velocity. The enhancement of the drift velocity of electrons in the channel is restricted by the transferred-electron effect, for example, various scattering processes. Equation (13) shows that the approximate expression of drift velocity, which has been discussed above, is able to incorporate the processes of electronic scattering,[18] and the results obtained from Eq. (13) are consistent with the Monte–Carlo simulation results, which were given by Refs. [16] and [22] respectively. Therefore, the drift velocity has a saturation region when the applied voltage V_{ds} is above a fixed value.

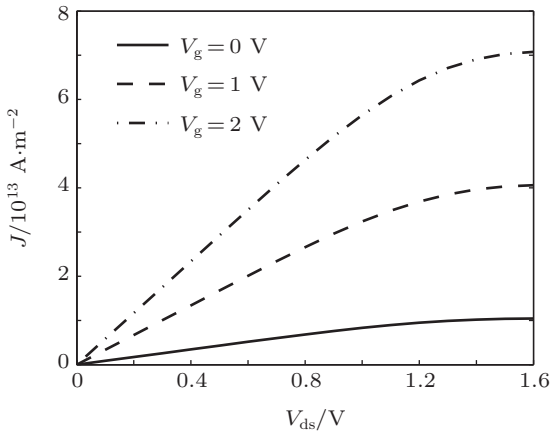


Fig. 3. The properties of J–V under gate biases of 0 V, 1 V, and 2 V.

The confinements of the current densities in the growth direction of the two materials under drain voltages of 0.5 V, 1.0 V, and 1.5 V, which indicate that a higher drain voltage will induce a higher current density in the central channel, are shown in Fig. 4. The current density is restricted in a narrow layer with a width of 5 nm, near the interface of the two materials. As mentioned above, since there are a large number of positive charges in the heterointerface of the two materials for the strong piezoelectric and spontaneous polarization fields existing in the $Al_{0.3}Ga_{0.7}N$/GaN heterostructure, electrons are driven to the area near the interface and then confined

into the triangular potential well, which makes up a 2DEG in this region.[9] From the self-consistent solution given by thr Shchrödinger and Poisson equations, we can derive the distribution of the density of the 2DEG which is restricted in a layer about 4 nm–5 nm in the potential triangular well near the heterointerface of the two materials.[24] Moreover, J–V properties of the $Al_{0.3}Ga_{0.7}N/GaN$ high electron mobility transistor are related to the density in the 2DEG channel, which can be seen from Eq. (3). Therefore, the confinement of the density distribution in the 2DEG channel determines the distribution of the current density, which is shown in Fig. 4.

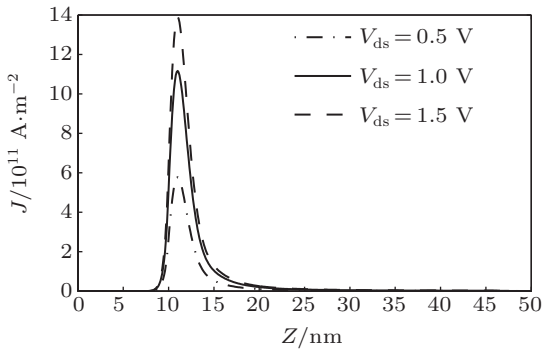


Fig. 4. Distributions of current density versus z position, which is the growth direction of the materials, under drain voltages of 0.5 V, 1.0 V, and 1.5 V.

4. Conclusion

In this paper, we obtained the J–V characteristics of the $Al_{0.3}Ga_{0.7}N/GaN$ high electron mobility transistor with an approach in which we considered the electronic microscopic characteristics of the 2DEG in a triangular potential well. In the frame of the self-consistent solution, we solve the Schrödinger and Poisson equations for the finite triangle-shaped quantum well, which forms the 2DEG at the $Al_{0.3}Ga_{0.7}N/GaN$ heterointerface. We use an approximate drift-velocity model in order to be able to incorporate the scattering processes of electrons and derive the relationship between current density and drain voltage. Our results show that the J–V characteristics of the HETM depend on the electronic properties at the two lowest subband energy levels, and the gate bias can provide an efficient way to control the J–V relation of HETM. From the distribution of the electronic probability density, it is indicated that the electronic current is confined only in a narrow channel about 5 nm, and the current density is up to about 10^{13} A/m^2. In addition, a current density of 7×10^{13} A/m^2 passing through the 2DEG channel with a 2DEG density of above 1.2×10^{17} m^{-2} under a drain voltage $V_{ds} = 1.5$ V at room temperature, the barrier thickness L_b should be more than 10 nm and the gate bias must be higher than 2 V.

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