A Deterministic Multi-Subband Boltzmann Transport Equation Solver for GaN Based HEMTs

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***Abstract*—A high electron mobility transistor based on a GaN channel is simulated by using a deterministic Boltzmann transport equation solver. In order to verify the physical soundness of the scattering mechanisms, first, a mobility calculator has been implemented. Phonon-limited electron mobility is calculated for one-dimensional heterostructure in the low field regime. For GaN based HEMTs, the two-dimensional Poisson equation and the one-dimensional Schrödinger equation along the confinement direction are considered. The transport of electrons in the non-equilibrium state is determined by solving the Boltzmann equation expanded with the Fourier harmonics in a self-consistent manner. The polar optical phonon is considered to explain the scattering of the system and the Pauli principle is also included. The Boltzmann equation is implemented for the total energy space with H-transformation. Without assistance from the momentum-based equation, the direct bias ramping from the equilibrium solution can be performed.**

***Index Terms*—Boltzmann transport equation; Self-consistent simulation; Polar optical phonon; GaN; HEMT**

I. Introduction

The drift-diffusion (DD) model has been widely used for simulation of semiconductor devices [1]. However, in modern nanoscale devices, prediction through the conventional DD model becomes difficult and more calibration is required [2]. The approximations adopted in deriving the DD model are no longer valid and it is necessary to solve the Boltzmann equation directly. Recently, the deterministic Boltzmann equation solvers have gained significant research interest [3]–[14].

In a deterministic solver, the distribution function is usually expanded with basis functions. Either the kinetic energy space or the total energy space (H-space) can be used as the energy variable [8]. The maximum entropy dissipation scheme or the H-transformation scheme to solve the problem of numerical instability due to strong internal electric fields can give reliable results on DC characteristics [12]. Although these deterministic solvers have been extensively used in studying the silicon devices, its application to the GaN devices is seldom found [4], [5].

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In this work, we implement a deterministic multi-subband Boltzmann equation solver for GaN based high electron mobility transistors (HEMTs) in the H-space. In Sec.II, the numerical method is explained and the results are discussed in Sec.III. Finally, the conclusion is made in Sec. IV.

II. Numerical Method

A. Mobility Calculation

Prior to the implementation of the transport equation, the phonon-limited electron mobility in the one-dimensional heterostructure is calculated using the Kubo-Greendwood formula [15], [16].

$$\mu_{ij}^{\nu} = \frac{e}{\hbar^2}\frac{1}{k_B T}\frac{g_v}{N_\nu}\int \frac{dk}{(2\pi)^2}\tau^{\nu}\frac{\partial E_\nu}{\partial k_i}\frac{\partial E_\nu}{\partial k_j} f_0(E_\nu)[1 - f_0(E_\nu)], \tag{1}$$

where e is the elementary charge, $\hbar$ is the Planck constant divided by 2π, k_B is the Boltzmann constant, T is the lattice temperature, g_v is the degeneracy, N_ν is the subband inversion carrier density, E_ν is the energy dispersion, f_0 is the Fermi-Dirac distribution, and τ^ν is the momentum relaxation time.

In the mobility calculation, deformation potential, piezoelectric, and polar optical phonon scatterings are considered. The mobility is calculated as a function of the electron density and the lattice temperature. A static screening effect is additionally considered for more realistic results at high electron densities [17].

B. Transport Equation

The multi-subband Boltzmann equation solver has been implemented as a part of our in-house device simulation framework, G-Device [14], [18]. The two-dimensional Poisson equation, the one-dimensional Schrödinger equation perpendicular to the transport direction, and the one-dimensional multi-subband Boltzmann transport equation are applied. In the Poisson equation, the gate contact is placed on the Schottky barrier layer and the Dirichlet boundary condition is applied. For one-dimensional transport equation, the equilibrium distribution function is imposed to the two nodes at the both ends of the channel. The structural description of the boundary conditions is shown in Fig.1.

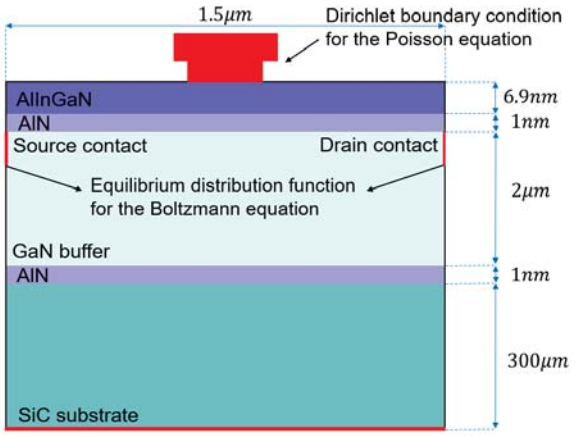

Fig. 1. Two-dimensional HEMT structure. The contacts with a Dirichlet boundary condition and the nodes with an equilibrium state distribution function are described.

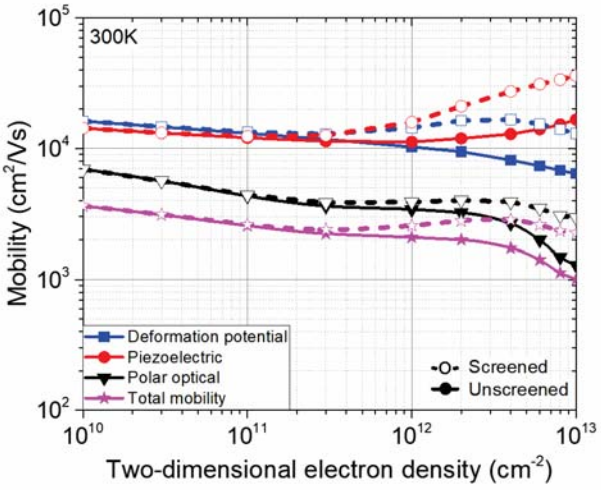

Fig. 2. Phonon-limited electron mobility as a function of the channel electron density.

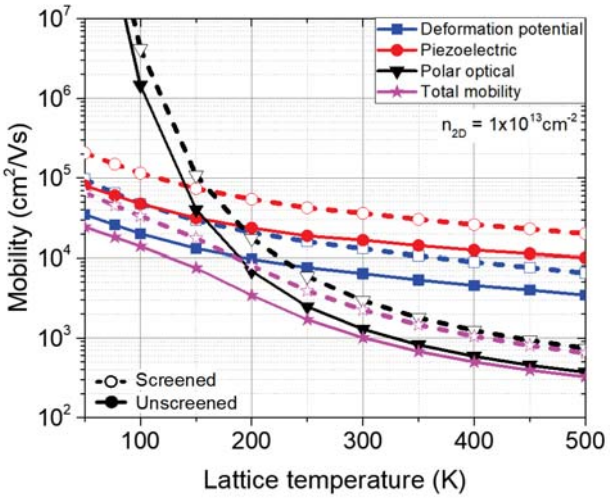

Fig. 3. Phonon-limited electron mobility as a function of the lattice temperature.

The Boltzmann equation is implemented in the H-space. The polar optical phonon scattering is taken into account and the Pauli principle is applied. The anisotropy of the polar optical phonon scattering can be considered by expanding the transition rate with the Fourier harmonics. Assuming that the transition rate from the initial state $\mathbf{k}$ to the final state $\mathbf{k}'$ is $S(x, \mathbf{k}'|\mathbf{k})$, the scattering integral term can be expressed as in-scattering and out-scattering [8]

$$\hat{S}_\nu\{f\} = \frac{1}{(2\pi)^2}\sum_{\nu'}\int \{(1-f(x,\mathbf{k}))S_{\nu,\nu'}(x,\mathbf{k}|\mathbf{k}')f(x,\mathbf{k}') - f(x,\mathbf{k})S_{\nu',\nu}(x,\mathbf{k}'|\mathbf{k})(1-f(x,\mathbf{k}'))\}\, d^2k'. \quad (2)$$

The transition rate for the polar optical phonon is given by

$$S^{POP}_{\nu',\nu}(x,\mathbf{k}'|\mathbf{k}) = \frac{2\pi}{\hbar}\frac{e^2\hbar\omega}{4}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\left(N(\hbar\omega)+\frac{1}{2}\mp\frac{1}{2}\right) \times \frac{F_{\nu,\nu'}(q)}{q}\delta(E_\nu(\mathbf{k})-E_{\nu'}(\mathbf{k}')\pm\hbar\omega), \quad (3)$$

where $\hbar\omega$ is phonon energy of the polar optical phonon, ϵ_∞ and ϵ_0 are the high frequency and static permittivities, respectively, and $N(\hbar\omega)$ is the phonon occupancy. The upper and lower signs in (3) refer to absorption and emission processes, respectively. Form-factor ($F_{\nu,\nu'}$) and change of the wavevector (q) are given by

$$F_{\nu,\nu'}(q) = \int\int \psi_\nu(z)\psi_{\nu'}(z)e^{-q|z-z'|}\psi_\nu(z')\psi_{\nu'}(z')dzdz',$$
$$q = |\mathbf{k}'-\mathbf{k}| = \sqrt{k'^2+k^2-2kk'\cos(\phi'-\phi)} \quad (4)$$

The Pauli principle and change of the wave vector make the expanded Boltzmann equation complicated.. The detailed form of the expanded Boltzmann equation is introduced in [8], [10]. In this work, we have dealt with the Boltzmann equation expanded up to the first order. However, the angular dependence of the transition rate of the polar optical phonon requires consideration of higher harmonic orders for more accurate simulation.

The relatively narrow band gap of the Schottky barrier material (AlInGaN) causes unintended hole density in the barrier layer at low gate biases. Therefore, a two-dimensional DD equation is solved for minority hole carriers.

III. Results and Discussion

Figs. 2 and 3 show the phonon-limited electron mobility of GaN in the low field regime. It can be confirmed that the polar optical phonon is the most dominant scattering mechanism at near room temperature and above. Therefore, the polar optical phonon is applied to determine the scattering mechanism of the Boltzmann solver for the GaN channel. Moreover, it is found that the screening effect is significant at high electron densities.

A two-dimensional HEMT having a GaN channel shown

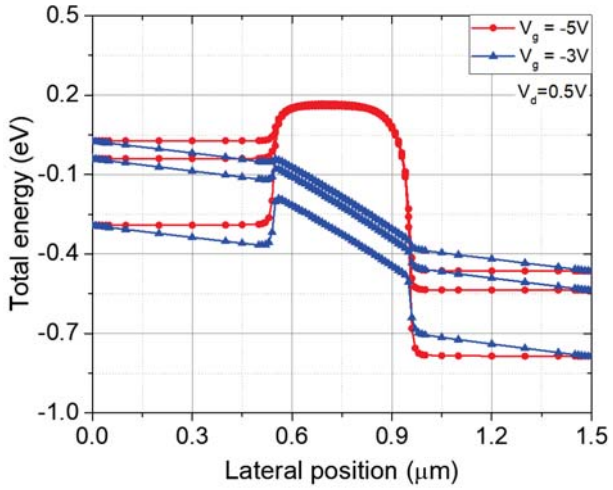

Fig. 4. Three lowest subband energies as functions of the lateral position for different gate biases at $V_d = 0.5V$.

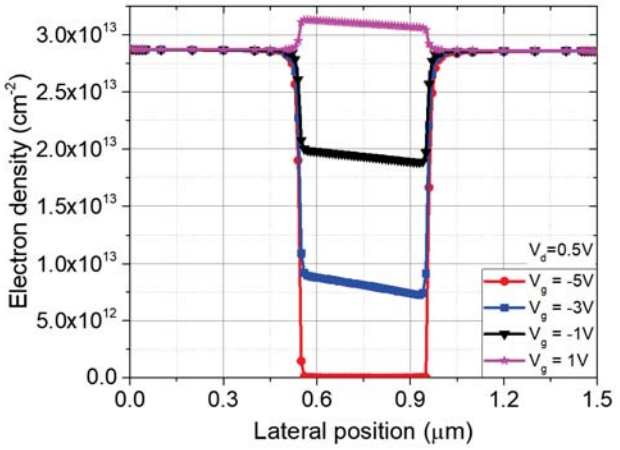

Fig. 5. Two-dimensional electron densities as functions of the lateral position for different gate biases at $V_d = 0.5V$.

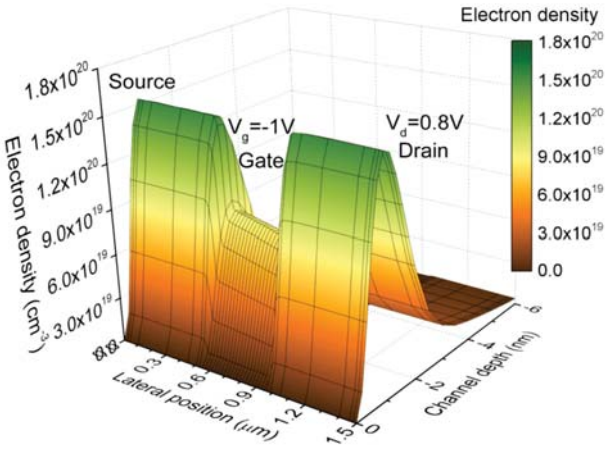

Fig. 6. Electron distribution in the GaN channel at $V_g = -1V$ and $V_d = 0.8V$.

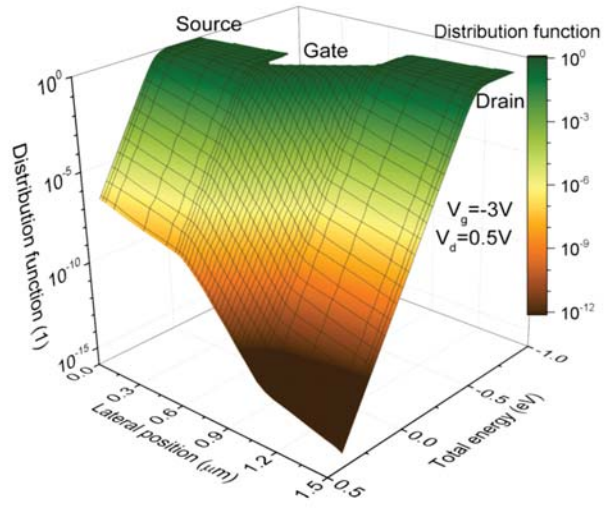

Fig. 7. Distribution function for the lowest subband in the GaN channel at $V_g = -3V$ and $V_d = 0.5V$.

in Fig. 1 is considered [19]. A two-dimensional electron gas (2DEG) in GaN is formed by spontaneous and piezoelectric polarization charges. Fig. 4 shows the three lowest subband energies at given bias points. At higher gate voltages, the lowest subband dominates the device characteristics. At lower gate voltages, the influence of higher subbands cannot be ignored because subbands are formed in a narrow energy space. Therefore, appropriate number of subbands should be considered. The electron sheet densities at the given bias points are shown in Fig. 5. Figs. 6 and 7 show the three dimensional electron density and the distribution function, respectively. The distribution function can be simulated over several orders of magnitude. Figs. 8 and 9 show the input and output characteristics of the GaN HEMT. It is noted that the output curves in Fig. 9 are calculated by performing a direct ramping of the drain voltage without any help from the momentum-based equations such as the DD model. It demonstrates the numerical robustness of our implementation.

IV. Conclusion

A deterministic multi-subband Boltzmann equation solver has been implemented for GaN based HEMTs. Phonon-limited electron mobility for GaN is calculated and the polar optical phonon scattering is applied to the Boltzmann solver. It is expected that a deterministic multi-subband Boltzmann solver can be used as a valuable tool for determining the DC characteristics in the nanoscale devices. Its numerical robustness plays a critical role in implementing the transient simulation capability.

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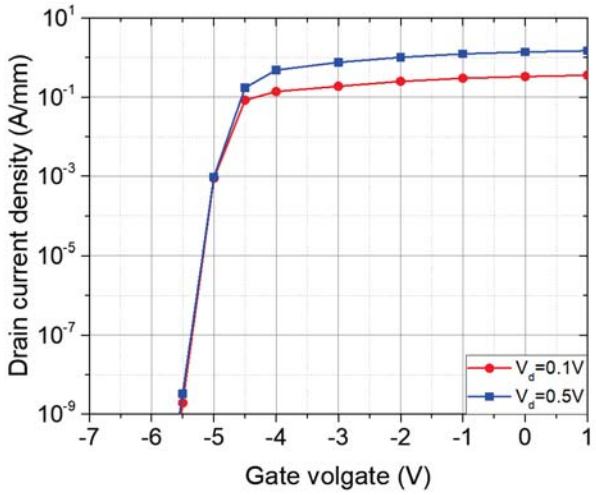

Fig. 8. Input characteristic for $V_d = 0.1V, 0.5V$.

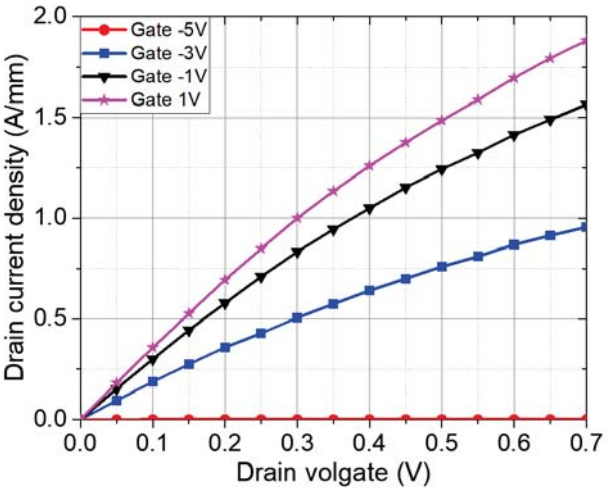

Fig. 9. Output characteristic for $V_g = -5V, -3V, -1V, 1V$.

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