Mobility of a two-dimensional electron gas in the AlGaN/GaN heterostructure: simulation and analysis

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Abstract. At temperatures higher than the room temperature, a two-dimensional electron gas (2DEG) formed at the AlGaN/GaN heterointerface can be characterized by the three dominant scattering mechanisms: acoustic deformation potential, polar acoustic phonon and polar optical phonon scatterings. An analytical model describing the 2DEG mobility limited by these scattering mechanisms as a function of the carrier concentration and the temperature was developed and integrated into a device simulator package using a C language interpreter. The model should be useful for heterostructure device simulators such as Blaze.

1. Introduction

Gallium nitride (GaN) is a binary III/V semiconductor with a wide band gap of 3.4 eV, which affords it outstanding properties for applications in high power, high frequency and optoelectronic devices. The excellent breakdown and reasonable transport characteristics of GaN are made full use of in heterojunction field-effect transistors or high electron mobility transistors (HEMTs), which are currently the most widespread electronic nitride devices. The HEMT is a field-effect transistor, incorporating a junction between two materials with different band gaps, i.e. heterojunction, to confine electrons to a triangular quantum well. As a result, the electrons are free to move in two dimensions but tightly confined in the third, thus forming a two-dimensional electron gas (2DEG). Figure 1 illustrates the conduction band edge (E_c) diagrams of the aluminium gallium nitride (AlGaN)/GaN heterostructure at absolute zero and at a temperature (T) above 0 K. The density in the 2DEG is determined by the conduction band edge and the Fermi level (E_F). Optimally only one of the quantized levels lies below the Fermi level. As the carriers in the triangular well are separated from the donors in the AlGaN layer by a thin space layer, which decreases the impurity scattering [1], the 2DEG exhibits a very high mobility.

Analyzing III/V semiconductors and devices with position-dependent band structures is complicated by the lack of a thorough approach to modeling, as the development of III/V materials has routinely trailed the advanced silicon technology. The electrical characterization of HEMTs requires accurate mobility models for carriers both in a bulk material layer and in a 2DEG. Popular heterostructure device simulator packages such as Blaze, however, do not include built-in 2DEG mobility models. In this paper, we develop and integrate into a device simulator using a C language interpreter an analytical model describing the 2DEG mobility limited by three dominant scattering mechanisms: acoustic deformation potential, polar acoustic phonon and polar optical phonon scatterings.

2. Structure

A two-dimensional schematic representation of the AlGaN/GaN HEMT structure, the electrical behavior of which is simulated using the developed 2DEG mobility model, is shown in figure 2. It consists of a 1.5 μm GaN buffer layer, a 20 nm $Al_{0.21}G_{0.79}aN$ barrier layer and 6 μm silicon nitride (Si_3N_4) passivation layer. The thickness and the length of the gate are equal to 3 μm and 0.5 μm, respectively. The source-to-gate and the gate-to-drain distances are 1 μm and 3.5 μm. The scale factor representing the third dimension in two-dimensional simulations equals to 150 μm. The thickness of the sapphire (Al_2O_3) substrate is 100 μm.

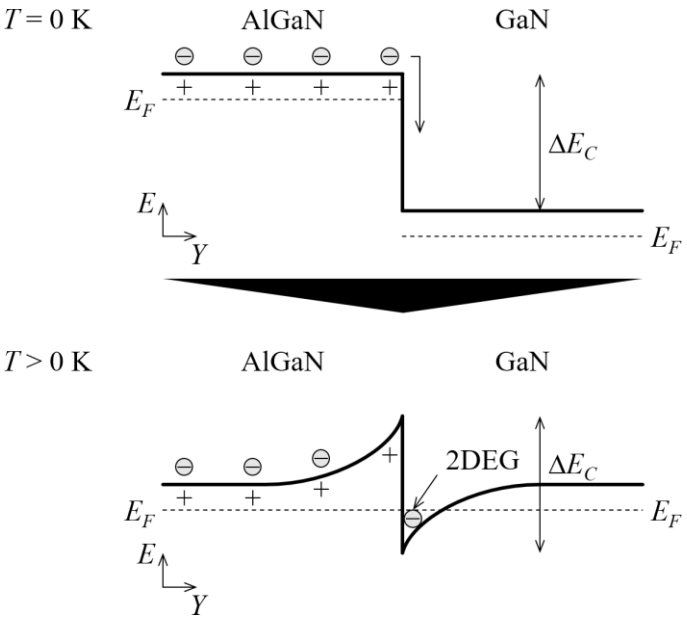

Figure 1. Conduction band edge diagrams of the AlGaN/GaN heterostructure at absolute zero and at a temperature above 0 K.

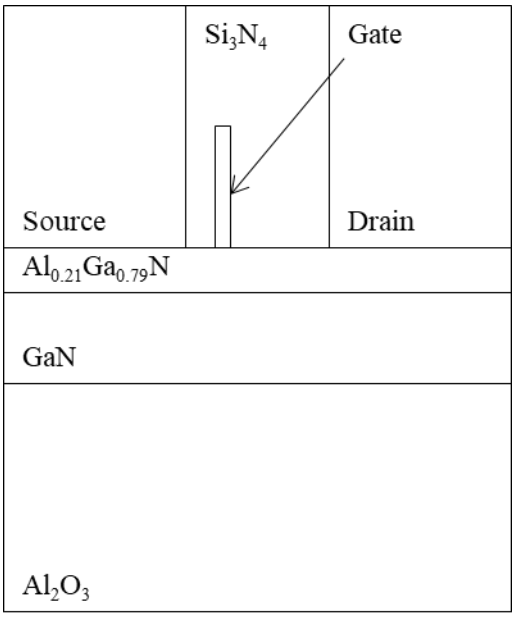

Figure 2. AlGaN/GaN HEMT structure.

3. Two-dimensional electron gas mobility model

At temperatures higher than the room temperature, a 2DEG formed at the AlGaN/GaN heterointerface can be characterized by the three dominant scattering mechanisms: acoustic deformation potential, polar acoustic phonon and polar optical phonon scatterings. As was noted previously, the impurity scattering is relatively low due to the space layer and is not accounted for in the mobility model.

The momentum relaxation time due to the acoustic deformation potential scattering is calculated as follows [1]:

$$\tau_{ADP} = \frac{\hbar^3 v_l^2 \rho b}{m\kappa T \varphi_{AD}^2}, \tag{1}$$

where $\hbar$ is the reduced Planck constant, v_l is the velocity of longitudinal acoustic phonon, ρ is the density, m is the effective mass, κ is the Boltzmann constant and φ_{AD} is the acoustic deformation potential.

In equation (1) b is the effective width of the 2DEG, which is defined as the double average distance of the electronic wave function from the heterointerface into GaN for the 0^{th} subband (z_0). According to Lee *et al.* [1], z_0 equals approximately to the distance from the heterointerface to the intersection of the conduction band edge and the Fermi level. Our simulations of AlGaN/GaN HEMTs using a self-

consistent coupled Schrodinger-Poisson model reveal that z_0 for a 2DEG density (n) of 10^{16} m^{-2} equals to 4 nm. In that case, the expression for b is given by

$$b = 2z_0 = 2\times 4\times 10^{-9}\left(\frac{10^{16}}{n}\right)^{\frac{1}{3}}. \tag{2}$$

The momentum relaxation time due to the polar acoustic phonon (piezoelectric) scattering mechanism is calculated as follows [2]:

$$\tau_{PE} = \frac{\pi}{q^2}\frac{\varphi_{AD}^2}{h_{14}^2}\frac{q_F}{b}\left(\frac{9}{32}+\frac{13}{32}\left(\frac{v_l}{v_t}\right)^2\frac{\Gamma_t}{\Gamma_l}\right)^{-1}\tau_{ADP}, \tag{3}$$

where q is the elementary charge, h_{14} is the piezoelectric constant and v_t is the velocity of transverse acoustic phonon.
In equation (3), q_F is the wave vector on the Fermi surface determined by

$$q_F = (2\pi n)^{\frac{1}{2}}. \tag{4}$$

The parameters Γ_l and Γ_t are defined by

$$\Gamma_l = \left(\left(\frac{4\gamma_l}{3\pi}\right)^2+1\right)^{\frac{1}{2}}, \tag{5}$$

$$\Gamma_t = \left(\left(\frac{4\gamma_t}{3\pi}\right)^2+1\right)^{\frac{1}{2}}, \tag{6}$$

where γ_l and γ_t are determined by

$$\gamma_l = \frac{2\hbar v_l q_F}{\kappa T}, \tag{7}$$

$$\gamma_t = \frac{2\hbar v_t q_F}{\kappa T}. \tag{8}$$

The momentum relaxation time due to the polar optical phonon scattering is calculated as follows [3]:

$$\tau_{POP} = \frac{4\hbar^2\pi\kappa_\varepsilon\varepsilon\left(1-5\frac{V_T}{E_g}\right)}{qm\left(2qmE_{POP}\left(1+\frac{E_{POP}}{E_g}\right)\right)^{\frac{1}{2}}N_P}, \tag{9}$$

where ε is the dielectric constant, V_T is the thermal voltage, E_g is the band gap and E_{POP} is the polar optical phonon energy.
In equation (9), κ_ε is the coupling constant:

$$\kappa_\varepsilon = \left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right)^{-1}, \tag{10}$$

where ε_∞ and ε_0 are the relative permittivity at high and low frequency, respectively.

The parameter N_p is the phonon Planck function:

$$N_P = \left(\exp\left(\frac{E_{POP}}{V_T} \right) - 1 \right)^{-1}. \quad (11)$$

The relation between the *i*-mobility limited by one scattering mechanism and the corresponding *i*-momentum relaxation time is

$$\mu_i = \frac{q}{m} \tau_i. \quad (12)$$

The overall 2DEG mobility limited by the three scattering mechanisms is calculated using Matthiessen's rule:

$$\frac{1}{\mu} = \frac{1}{\mu_{ADP}} + \frac{1}{\mu_{PE}} + \frac{1}{\mu_{POP}}. \quad (13)$$

4. Results

In figures 3(a, b, c, d), the temperature dependences of the 2DEG mobility limited by each of the three scattering mechanisms and the overall mobility are presented for different 2DEG densities.

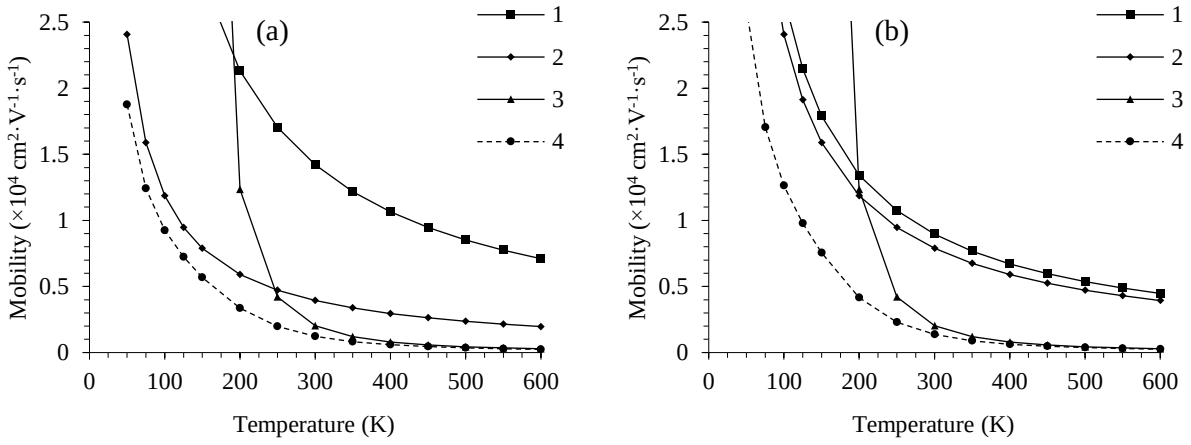

Figure 3(a, b). 2DEG mobility vs temperature for $n = 1 \cdot 10^{12}$ cm^{-2} **(a)** and $4 \cdot 10^{12}$ cm^{-2} **(b)**: 1 – acoustic deformation potential scattering; 2 – polar acoustic phonon scattering; 3 – polar optical phonon scattering; 4 – overall mobility.

As can be seen from the charts, if $n = 1 \cdot 10^{12}$ cm^{-2}, the acoustic deformation potential scattering mechanism has a minor impact on the 2DEG mobility at any temperatures. For instance, at the temperature of 600 K, μ_{ADP} equals to 7100 cm^2/(V·s), while the overall mobility is 241 cm^2/(V·s). When the electron concentration is raised, this mechanism increases its influence on the total mobility. In case of $n = 1 \cdot 10^{13}$ cm^{-2}, μ_{ADP} reaches the value of 3296 cm^2/(V·s) at $\mu = 253$ cm^2/(V·s). At the same time, the polar acoustic phonon scattering reduces its influence on the total mobility (μ_{PE} changes from the value of 1967 cm^2/(V·s) to 6228 cm^2/(V·s)), when the electron concentration is increased, but remains considerable at the whole temperature range.

At temperatures higher than the room temperature, the mobility of the 2DEG with any carrier concentration is governed predominantly by the polar optical phonon scattering mechanism [4] and (9) may be used as a rough approximation expression for the mobility at high temperatures.

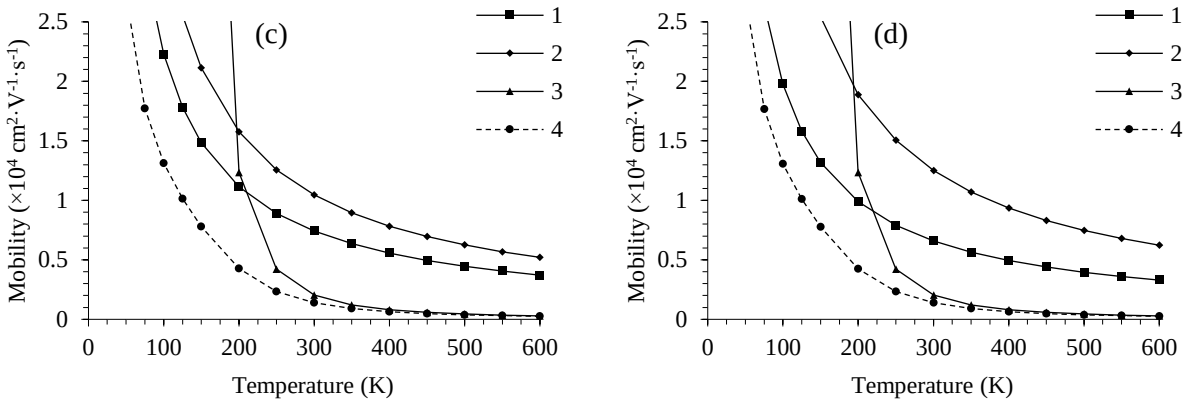

Figure 3(c, d). 2DEG mobility vs temperature for $n = 7 \cdot 10^{12}$ cm^{-2} **(c)** and $1 \cdot 10^{13}$ cm^{-2} **(d)**: 1 – acoustic deformation potential scattering; 2 – polar acoustic phonon scattering; 3 – polar optical phonon scattering; 4 – overall mobility.

In figure 4, the drain current vs drain voltage characteristics of the simulated AlGaN/GaN HEMT are presented. For comparison, one curve is calculated with the electron mobility in the device channel equal to 400 cm^2/(V·s), a value commonly obtained for bulk GaN [5], and another is calculated using the developed model. The temperature is constant (300 K) and the gate voltage is 0 V.

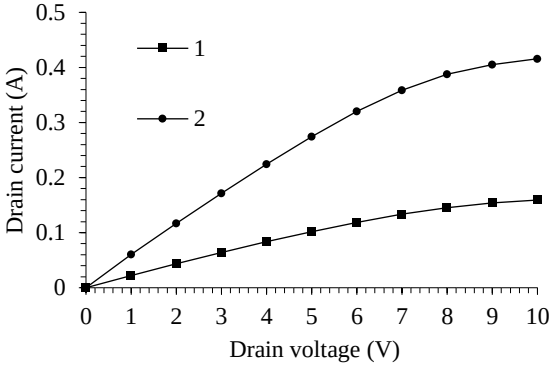

Figure 4. Output characteristics of the simulated AlGaN/GaN HEMT: 1 – bulk mobility model; 2 – developed 2DEG mobility model.

The calculated 2DEG mobility under the gate equals to 1378 cm^2/(V·s). We suppose that the developed model can be useful for heterostructure device simulators such as Blaze.

Acknowledgments
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