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Two-dimensional electron transport in AlGaN/GaN heterostructures

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ABSTRACT

We present a theoretical study of electron transport properties of two-dimensional electron gas in AlGaN/GaN heterostructures. By assuming a drifted Fermi–Dirac distribution and taking into account all major scattering mechanisms, including polar optical and acoustic phonons, background impurities, dislocation and interface roughness, the momentum- and energy-balance equations derived from Boltzmann equation are solved self-consistently. The dependence of the electron drift velocity and electron temperature as a function of the applied electric field are obtained and discussed.

1. Introduction

Over the past decade, there has been increasing interest in the study of GaN material and GaN-based electronic and optoelectronic devices. Due to its large direct bandgap energy, large saturation velocity, high breakdown voltage and high temperature stability, GaN is an ideal material for a variety of electronic and optoelectronic applications, such as light-emitting diodes, blue lasers, transistors operating in a wide range frequency and high power [1–4]. Many device operations rely on the electron transport properties, therefore experimental and theoretical studies on electric field dependent drift velocity in GaN material and related heterostructures are extremely important.

Electron transport properties in GaN material and GaN-based nanostructures have been calculated by many authors using the Monte-Carlo (MC) technique [5–7] and the phenomenological velocity-field model [8]. The MC technique is a numerical solution to the Boltzmann equation with less approximations and has become a powerful tool in the treatment of semiconductor transport and device modeling. However, this numerical method is considerably CPU consuming, and has intrinsic shortcomings in offering physical insights and systematic analyses. Besides the MC method and the phenomenological model, it is known that the balance-equation approach is an effective method in studying the linear and nonlinear response of a semiconductor device to the dc and ac electric field applied [9–11]. Generally speaking, the balance-equation approach contains mass balance, momentum/force balance, and energy balance. In this paper, we investigate the transport characteristics of a two-dimensional electron gas (2DEG) in an AlGaN/GaN heterostructure by using the momentum- and energy-balance equations which are derived from the Boltzmann equation. In this approach, we avoid the difficulties in solving directly the Boltzmann equation. The electric field dependence of the electron drift velocity, the mobility and electron temperature are calculated at different lattice temperatures. Different scattering mechanisms are considered in the model and the effects on transport are discussed.

2. Theoretical approach

2.1. Electronic transition rates

In this work, we consider a 2DEG in an AlGaN/GaN heterostructure whose growth-direction is taken along the z-axis with a confining potential $U(z)$ and electron transport occurs in the xy-plane. Considering the electron interactions with impurities and phonons in the heterostructure, the Hamiltonian to describe such a system can be written as

$$H = H_0 + H_{e-i} + H_{e-p}. \quad (1)$$

Here, $H_0 = \mathbf{P}^2/2m^* + U(z)$ is the electron Hamiltonian, m^* is the electron effective mass, $\mathbf{P} = (p_x, p_y, p_z)$ with $p_x = -i\hbar\partial/\partial x$ is the momentum operator along the x-direction, and H_{e-i} and H_{e-p} are the electron–impurity interaction and electron–phonon

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interaction Hamiltonian, respectively. In the usual effective mass approach, the electron wavefunction and energy spectrum with regarding to H_0 can be written, as

$$|n,\mathbf{k}\rangle = \Psi_{n\mathbf{k}}(\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{r}}\psi_n(z), \tag{2}$$

and

$$E_n(\mathbf{k}) = \hbar^2 k^2/2m^* + \varepsilon_n, \tag{3}$$

where n is the index for the nth electronic subband along the growth direction, $\mathbf{k}=(k_x,k_y)$ is the electron wavevector in the xy-plane, and $\mathbf{R}=(\mathbf{r},z)=(x,y,z)$. The electron wavefunction $\psi_n(z)$ and the nth subband energy ε_n are determined by

$$[-(\hbar^2/2m^*)d^2/dz^2 + U(z) - \varepsilon_n]\psi_n(z) = 0. \tag{4}$$

We take the electron–phonon interaction and electron–impurity interaction as perturbations. For electron interaction with bulk-like phonons, the Hamiltonian takes a form

$$H_{e-p} = \sum_{\mathbf{q}_z}[V_{\mathbf{Q}}a_{\mathbf{Q}}e^{i(\mathbf{Q}\cdot\mathbf{R}+\omega_Q t)} + V^*_{\mathbf{Q}}a^\dagger_{\mathbf{Q}}e^{-i(\mathbf{Q}\cdot\mathbf{R}+\omega_Q t)}], \tag{5}$$

where $\mathbf{Q}=(\mathbf{q},q_z)=(q_x,q_y,q_z)$ is the phonon wavevector, $(a^\dagger_{\mathbf{Q}},a_{\mathbf{Q}})$ are the canonical conjugate coordinates of the phonon system, $V_{\mathbf{Q}}$ is the electron–phonon interaction coefficient, and ω_Q is the phonon frequency. Applying the electron wavefunction (Eq. (2)) and energy spectrum (Eq. (3)) to the Fermi's golden rule, the electronic transition rate induced by phonon scattering processes is obtained as

$$W^{ep}_{nn'}(\mathbf{k},\mathbf{k}') = \frac{2\pi}{\hbar}\sum_{\mathbf{q}_z}\begin{bmatrix} N_Q \\ N_Q+1 \end{bmatrix}|V_{\mathbf{Q}}|^2 G_{nn'}(q_z)\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\delta[E_n(\mathbf{k}) - E_{n'}(\mathbf{k}') \pm \hbar\omega_Q], \tag{6}$$

where $\mathbf{q}=(q_x,q_y)$ is the change of the electron wavevector during an electron scattering event, and the upper (lower) case refers to absorption (emission) of a phonon, $N_Q=(e^{\hbar\omega_Q/k_BT}-1)^{-1}$ is the phonon occupation number, and $G_{n'n}(q_z)=\left|\int dz\,\psi^*_{n'}(z)\psi_n(z)e^{iq_zz}\right|^2$ is the form factor for the electron–phonon interaction in a 2DEG system.

For electron–LO–phonon interaction, described by the Fröhlich Hamiltonian, we have [9]

$$|V_{LO}(\mathbf{Q})|^2 = 4\pi\alpha L_0(\hbar\omega_{LO})^2/Q^2, \tag{7}$$

with α the electron–LO–phonon coupling constant, $L_0=(\hbar/2m^*\omega_{LO})^{1/2}$ the polaron radius. The matrix elements $|V_{\mathbf{Q}}|^2$ for deformation potential, longitudinal piezoelectric and transverse piezoelectric scattering are given by [9]

$$|V_{DP}(\mathbf{Q})|^2 = \frac{E_D^2\hbar Q}{2\rho v_l}, \tag{8}$$

$$|V_{LP}(\mathbf{Q})|^2 = \frac{32\pi^2\hbar^2(eh_{14})^2}{\kappa^2\rho v_l}\frac{(3q_xq_yq_z)^2}{Q^7}, \tag{9}$$

and

$$|V_{TP}(\mathbf{Q})|^2 = \frac{32\pi^2\hbar^2(eh_{14})^2}{\kappa^2\rho v_t Q^5}(q_x^2q_y^2+q_y^2q_z^2+q_z^2q_x^2) - \frac{(3q_xq_yq_z)^2}{Q^2}, \tag{10}$$

Here, E_D is the deformation potential constant, ρ is the density, κ is the dielectric constant, h_{14} is the piezoelectric constant, and $v_l(v_t)$ is the longitudinal (transverse) sound velocity in GaN.

The electronic transition rate induced by impurity scattering processes is obtained as

$$W^{ei}_{nn'}(\mathbf{k},\mathbf{k}') = \frac{2\pi}{\hbar}|U_{nn'}(q)|^2\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\delta[E_n(\mathbf{k}) - E_{n'}(\mathbf{k}')], \tag{11}$$

with

$$|U_{nn'}(q)|^2 = \left[\frac{2\pi Ze^2}{\kappa(q+q_{TF})}\right]^2\int dz_a n_i(z_a)F_{nn'}(q,z_a), \tag{12}$$

where $n_i(z)$ is the impurity distribution along the growth direction, $q_{TF}=2m^*e^2/\kappa\hbar^2$ is the Thomas–Fermi wave vector, and $F_{nn'}(q,z_a)=\left|\int dz\,\psi^*_{n'}(z)\psi_n(z)e^{-q|z-z_a|}\right|^2$ is the form factor for electron–impurity scattering in a 2DEG system. In the present study, we consider an unintentionally doped AlGaN/GaN heterostructure, i.e., the ionized impurity scattering is mainly caused by the background impurities, which can be approximated as a uniform volume density N_I in the GaN region.

2.2. Momentum- and energy-balance equations

With the electronic transition rates, we apply the Boltzmann equation approach to study the electronic transport properties in a 2DEG system. In this study, we employ a semiclassic Boltzmann equation as the governing transport equation to reveal the effect of a driving electric field F_x applied along the x-direction. In the case of a degenerate statistics, the steady-state Boltzmann equation can be written as [12]

$$-\frac{eF_x}{\hbar}\frac{\partial f_n(\mathbf{k})}{\partial k_x} = \sum_{n',\mathbf{k}'}[F_{n'n}(\mathbf{k}',\mathbf{k}) - F_{nn'}(\mathbf{k},\mathbf{k}')], \tag{13}$$

where $F_{nn'}(\mathbf{k},\mathbf{k}')=f_n(\mathbf{k})[1-f_{n'}(\mathbf{k}')]W_{nn'}(\mathbf{k},\mathbf{k}')$, $f_n(\mathbf{k})$ is the momentum-distribution function for an electron at state $|n,\mathbf{k}\rangle$, and $W_{nn'}(\mathbf{k},\mathbf{k}')$ is the electronic transition rate from state $|n,\mathbf{k}\rangle$ to state $|n',\mathbf{k}'\rangle$ induced by scattering.

In the presence of the driving electric field and scattering centers, the distribution function can be determined by the Boltzmann equation, and therefore the interested physical quantities can be calculated. We assume that the momentum distribution in a high density 2DEG system can be described by a Fermi–Dirac statistics through

$$f_n(\mathbf{k}) \simeq f(E_n(\mathbf{k}-m^*\mathbf{v}_n/\hbar),T_n), \tag{14}$$

where the momentum is shifted due to the presence of the driving field F_x, $\mathbf{v}_n=(v_n,0,0)$ is the average drift velocity of the electrons in the nth subband, T_n is the electron temperature for electrons in the nth subband, and $f(x,T_n)=[e^{(x-\mu^*)/k_BT_n}+1]^{-1}$ with μ^* being the Fermi energy of the 2DEG system, which is determined by the electron density $N=g_s\sum_{n,\mathbf{k}}f_n(\mathbf{k})$, where $g_s=2$ accounts for the spin degeneracy.

It is known that there is no simple and analytical solution to the Boltzmann equation (Eq. (13)) with the electronic transition rate given by Eqs. (6) and (11). Here, we apply the usual balance-equation approach to solve the problem [11]. For the first moment, the momentum-balance equation can be derived by multiplying $g_s\sum_{\mathbf{k}}k_x$ to both sides of Eq. (13), which reads

$$eF_xN_n = 2\hbar\sum_{n',\mathbf{k}',\mathbf{k}}(k_x'-k_x)f_n(\mathbf{k})[1-f_{n'}(\mathbf{k}')]W_{n,n'}(\mathbf{k},\mathbf{k}'), \tag{15}$$

where $N_n=g_s\sum_{\mathbf{k}}f_n(\mathbf{k})$ is the electron density in the nth subband. For the second moment, the energy-balance equation can be derived by multiplying $g_s\sum_{\mathbf{k}}E_n(\mathbf{k})$ to both sides of Eq. (13), which reads

$$eF_xN_nV_n = 2\sum_{n',\mathbf{k}',\mathbf{k}}[E_n(\mathbf{k}')-E_n(\mathbf{k})]f_n(\mathbf{k})[1-f_{n'}(\mathbf{k}')]W_{n,n'}(\mathbf{k},\mathbf{k}'). \tag{16}$$

For simplicity, we consider the momentum loss due to dislocation and interface roughness scattering by means of their average momentum relaxation time, which reads

$$eF_x = m^*v/\tau_j, \tag{17}$$

where j stands for a specific scattering mechanism.