Polar charges effect on multisubband electron mobility in the semiparabolic quantum wells based on AlN/AlGaN/AlN

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Abstract. This work presents multisubband electron mobility in the polarization semi-parabolic quantum wells (SPQWs) AlN/Al\textsubscript{x}Ga\textsubscript{1-x}N/AlN. First, a theory of multisubband mobility between the lowest two subbands under a uniform external electric field is studied. By using the variation method, the one-dimensional Poisson and Schrödinger equations have been solved within a finite potential barrier model and a bent band figured by all confinement sources (realistic model). Then, we computed and discussed about the effective confining potential profile, the wave function and multisubband mobility. Our result shows that the positive interface polarization charges effect on the distribution of the two-dimensional electron gas (2DEG) in SPQWs so it has great influences on multisubband mobility.

1. Introduction
In recent years, asymmetric quantum well structures have been continued to be a great deal model for study properties of low dimensional structures [1-4]. These structures also exhibit interesting applications in electronic and optoelectronic devices, such as high electron mobility transistor (HEMT), semiconductor lasers, optical switching, infrared photodetectors, and so on [5-9]. In recent work, effect of asymmetry on the electronic properties such as electron transport and spin transport in quantum wells has also been studied by applying an external electric field perpendicular to the interface plane of the structure [10-12]. Attempts have been made to study the optical properties of asymmetric quantum wells [14].

Literature survey shows that the research in this field is often based on solving Schrödinger equation to find the wave functions and analyzing numerical results. Electron mobility are obtained and the effects of the changing quantum well parameters are investigated. In this way one must restrict himself to well-known infinite potential wells such as parabolic and semi-parabolic QWs [13-15]. It should be noted that the infinite potential wells are not physically feasible. However progress in computational physics with high accuracy permits us to investigate the finite potential wells [16], which are important theoretically and experimentally. Few works have also been reported on electron transport in GaAs/AlGaAs and strained layer asymmetric quantum well structures [17, 18]. In these structures the electron mobility is studied by considering lowest subband occupancy. However, in a system, where more than...
one subband is occupied, the intersubband effects play a major role on the subband mobility [13-16]. Despite the fact that there were some important studied results about the multisubband electron mobility in GaN quantum wells but a systematic study on AlN/Al_{x}Ga_{1-x}N/AlN heterostructures (HSs) is still lacking. In this work, we investigate the effects of the widths of the QWs, the aluminum concentration in Al_{x}Ga_{1-x}N and the strength of the applied electric field on the multisubband electron mobility of the polarization SPQWs based on AlN/Al_{x}Ga_{1-x}N/AlN HSs. The confinement potential form of the studied system is shown schematically in Figure 1. Especially, we have known that polarization is an important property of a nitride and oxide-based heterostructures [19, 20]. These HSs possess a very high (a real) density of polarization charges bound on the interface (σ ~ 10^{13} cm^{-2}). For formation of 2DEG in a polar HS, interface polarization charges take a double role: they are a source to supply carriers (electrons) into the sample, but they also are a source to confine the carriers along the growth direction. So, the polarization confinement effect has to be considered carefully.

![Figure 1. Schematic diagram for a semi-parabolic quantum well.](image)

To do end, the variational method [21, 22] is employed to solve the one-dimensional Poisson and Schrödinger equations for the SPQWs. Then the results are used to calculate the multisubband electron mobility by combining the results of Poisson and Schrödinger to scatterings due to interface roughness and alloy disorder. This paper is organized as follows. In Section 2, we present the theoretical results about how to find the wave functions and eigenvalues of electron in QWs, write down the formalism of the multisubband electron mobility of the system. Section 3 is dedicated to the numerical results for the confining potential forms and the distribution of electrons in the SPQWs. Also, we have investigated the changes of the multisubband electron mobility for the SPQWs. Finally, the conclusions are given in Section 4.

2. Theoretical calculation

2.1. Confining potentials

The two-dimensional electron gas (2DEG) in the semi-parabolic wells is described by the variational wave function [15]:

\[ \psi_i(z) = A_i e^{-\alpha_i z^2} H_{2i+1}[(2\alpha_i + 1)] \]  

(1)

A_i is the normalization constant, \( \alpha_i \) is the typical parameter of band bending. \( H_{2i+1}(2\alpha_i + 1) \) denote the Hermite polynomials. The quantum confinement along the z direction is determined by the following Hamiltonian:

\[ H = T + V_{tot}(z) \]  

(2)
where $T$ is the kinetic energy, and $V_{\text{tot}}(z)$ is the overall confining potential.

Carrier confinement in a polar modulation-doped HS is determined by all confining sources located along the growth direction ($z$-axis): potential barrier, interface polarization charges, Hartree potential and electric field potential induced by ionized impurities and 2DEG:

$$
V_{\text{tot}}(z) = V_b(z) + V_\sigma(z) + V_H(z) + V_{\text{ex}}(z) + V_F(z)
$$

(3)

First, for the potential barrier with a finite height $V_0$, it can be written:

$$
V_b(z) = \begin{cases} 
\frac{V_0}{L^2}z^2 & 0 \leq z \leq L \\
V_0 & z < 0; z > L
\end{cases}
$$

(4)

It is well known [20, 23] that due to piezoelectric and spontaneous polarizations in a nitride-based strained HS there exist positive polarization charges bound on the interface. These charges create a uniform normal electric field with the potential given by:

$$
V_\sigma(z) = \frac{2\pi e}{\varepsilon} |\sigma| z
$$

(5)

with $\sigma$ as the density of polarization charges. $\varepsilon$ is the average dielectric constant of the sample.

Next, the Hartree potential induced by the ionized donors and 2DEG in the HS. We consider the non-doping system, so $V_H = V_s$, $V_s(z)$ is confined potential electrons themselves. This is determined according to Poisson’s equation:

$$
\frac{d^2V_s(z)}{dz^2} = -\frac{4\pi e^2}{\varepsilon_a} N_i(z)
$$

(6)

Here, $N_s(z)$ is the bulk density of electron. It holds

$$
N_i(z) = n_i(z) |\psi(z)|^2
$$

(7)

$n_i$ is the number of electrons per unit area in the $i$th subband [19];

$$
n_i = \frac{m^* k_B T}{\pi \hbar^2} \ln \left[ 1 + \exp \left( \frac{E_{F_i} - E_i}{k_B T} \right) \right]
$$

(8)

with $m^*$ as the in-plane effective mass of the electron and Fermi level $E_{F_i}$ is given by:

$$
E_{F_i} = k_B T \ln \left[ \exp \left( \frac{\pi \hbar^2 n_i}{m^* k_B T} \right) - 1 \right]
$$

(9)

The potential by the electric field along the growth direction is given by:

$$
V_F(z) = |e| F z,
$$

(10)

where, $F$ is the strength of the applied electric field.

2.2. Total energy per electron in the two lowest subband

We now turn to the total energy per electron when the 2DEG occupying the lowest two subbands.

The expectation value of the Hamiltonian given by Eqs. (2) and (3) reads [21]:

$$
E_i = \langle T \rangle_i + \langle V_b \rangle_i + \langle V_\sigma \rangle_i + \langle V_s \rangle_i / 2 + \langle V_{\text{ex}} \rangle_i + \langle V_F \rangle_i,
$$

(11)
where $V_s$ is the value of $V_H$ for undoped systems, $V_{ex}$ is the exchange correlation interaction and has very small value so it is ignorable. Upon employing the above-derived analytic expressions for the individual confining potentials, we may easily calculate their expectation values with the lowest two subband wave function from Eq. (1). The average energies figuring in Eq. (11) are supplied below.

For the first state,

$$\langle T \rangle_1 = \frac{5\sqrt{\pi} \alpha_1 A_2^2 \hbar^2}{2m_z},$$  \hspace{1cm} (12)$$

$$\langle V_b \rangle_1 = \frac{V_0 A_2^2}{\alpha_1^2} \left( -4\alpha_1 + 3\sqrt{\pi} \alpha_1 \right) + \frac{V_0 A_2^2}{2L^2 \alpha_1^3} e^{-L^2 \alpha_1^2} \left[ -2 \left( 4 + L \alpha_1 (5 + 2L \alpha_1 (2 + L \alpha_1)) \right) + e^{L^2 \alpha_1^2} (8 + 5\sqrt{\pi} \text{Erf} [L \alpha_1]) \right] + \frac{V_0 A_2^2}{\alpha_1^2} \left[ 3\sqrt{\pi} \alpha_1 + 2e^{-L^2 \alpha_1^2} \alpha_1 (2 + L \alpha_1) - 3\sqrt{\pi} \alpha_1 \text{Erf} [L \alpha_1] \right],$$  \hspace{1cm} (13)$$

$$\langle V_s \rangle_1 = -\frac{2\pi e^2 A_1^4 n_1}{\varepsilon_a \alpha_1^2} \left( 24\pi + 31\sqrt{2\pi} \right),$$  \hspace{1cm} (15)$

$$\langle V_F \rangle_1 = \frac{4\sqrt{\pi} A_2^2 |e| F}{\alpha_1^2},$$  \hspace{1cm} (16)$$

and for the second state,

$$\langle T \rangle_2 = \frac{436\sqrt{\pi} \alpha_2 A_2^2 \hbar^2}{2m_z},$$  \hspace{1cm} (17)$$

$$\langle V_b \rangle_2 = \frac{V_0 A_2^2}{\alpha_2} \left( 344\sqrt{\pi} - 592 \right) + \frac{V_0 A_2^2}{L^2 \alpha_2^3} e^{-L^2 \alpha_2^2} \left[ 916\sqrt{\pi} e^{L^2 \alpha_2^2} \text{Erf} [L \alpha_2] - \left( 32L^7 \alpha_2^7 + 192L^6 \alpha_2^6 + 496L^5 \alpha_2^5 + 832L^4 \alpha_2^4 + 1216L^3 \alpha_2^3 + 1616L^2 \alpha_2^2 + 1832L \alpha_2 + 1616 \right) \right] + 1616 \right] + \frac{81V_0 A_2^2 e^{-L^2 \alpha_2^2}}{\alpha_2^2} \left[ \left( 43\sqrt{\pi} \alpha_2 e^{L^2 \alpha_2^2} + 2\alpha_2 \left( 2L^5 \alpha_2^5 + 12L^4 \alpha_2^4 + 29L^3 \alpha_2^3 + 40L^2 \alpha_2^2 + 42L \alpha_2 + 37 \right) \right) - 43\sqrt{\pi} \alpha_2 e^{L^2 \alpha_2^2} \text{Erf} [L \alpha_2] \right],$$  \hspace{1cm} (18)$$

$$\langle V_s \rangle_2 = \frac{3776\pi e A_2^2 \sigma}{\varepsilon_a \alpha_2^2},$$  \hspace{1cm} (19)$$

$$\langle V_s \rangle_2 = -\frac{2\pi e^2 A_1^4 n_2}{\varepsilon_a \alpha_1^2} \left( 726528\pi + 358351\sqrt{2\pi} \right),$$  \hspace{1cm} (20)$$

$$\langle V_F \rangle_2 = \frac{1056 \sqrt{\pi} A_2^2 |e| F}{\alpha_2^2}.$$  \hspace{1cm} (21)$$

2.3. The electron mobility

The electron mobility $\mu$ relation with the transport life time $\tau$ is given by:

$$\mu = \frac{e\tau}{m^*}.$$  \hspace{1cm} (22)
For multisubband with \( R \)th (AD-, SR-, PSR-...) scattering event, the electron mobility \( \mu^P \) can be written as
\[
\mu^P = \sum_i n_i \frac{n_i^R}{n_i} \tag{23}
\]

The total mobility \( \mu \) is calculated using Matthiessen relation [24]. When \( i = 1 \), we can write \( \tau_1 \) as
\[
\frac{1}{\tau_1} = B_{11} \tag{24}
\]

where \( B_{ij} \) is the intrasubband scattering rate matrix element. However, when we consider two subband \((n = 1, 2)\), \( \tau_1 \) and \( \tau_2 \) must have intersubband scattering rate matrix elements \( C_{ij} \) and \( D_{ij} \) [25, 26]:
\[
\frac{1}{\tau_1} = (B_{11} + C_{12}) (B_{22} + C_{21}) - D_{12} D_{21} \\
\frac{1}{\tau_2} = (B_{11} + C_{12}) (B_{22} + C_{21}) - D_{12} D_{21} \tag{25}
\]

here, \( B_{ii}, C_{ij} \) and \( D_{ij} \) are determined by [25, 26]:
\[
B_{ii} = m^* \left/ \left( \pi \hbar^3 \right) \int_0^\pi d\theta (1 - \cos \theta) \left| V_{ii}^R (q_{ii}) \right|^2 \\
C_{ij} = m^* \left/ \left( \pi \hbar^3 \right) \int_0^\pi d\theta \left| V_{ii}^R (q_{ij}) \right|^2 \tag{26}
\]
\[
D_{ij} = m^* \left/ \left( \pi \hbar^3 \right) \int_0^\pi \cos \theta \left| V_{ii}^R (q_{ij}) \right|^2 
\]

In this work, interface roughness scattering and alloy disorder scattering were considered.

Interface roughness scattering (PSR)

PSR scattering due to the potential induced by both normal surface roughness, or, strictly speaking, barrier roughness (position fluctuations of the potential barrier), \( V_{SR} \), and polarization roughness (position fluctuations of the polarization charges), \( V_{PR} \):
\[
V_{PSR} = V_{SR} + V_{PR} \tag{27}
\]

Scattering at rough interfaces can be severe if the 2DEG density is high, since the 2DEG tends to shift closer to the interface as the density increases. The roughness at heterojunction interfaces has been traditionally modelled by a Gaussian autocovariance function. However, in our research, surface roughness potential is determined as following [27]:
\[
\left| V_{ij}^{SR} (q_{ij}) \right|^2 = \pi \Delta^2 e^{-\frac{q_i^2 A^2}{4}} \left| \sum_{i,j'} \psi_i(z) \psi_j(z) e^{-\frac{1}{2} q_{ij}^2} \right|^2 \tag{28}
\]

Polarization is an important property of nitride- and oxide-based HSs. These HSs possess a very high density of polarization charges bound. It has been recently shown that these charges have a three-fold role similar to the ionized impurities. The polarization charges on a rough interface are a carrier supply source, a confining source, and a scattering mechanism for HSs. Therefore, it has become a key scattering and this project, we can consider polarization scattering potential as following [28-30]:
\[
\left| V_{ij}^{PR} (q_{ij}) \right|^2 = \pi \Delta^2 e^{-\frac{q_i^2 A^2}{4}} \left| \int_{-\infty}^{+\infty} \frac{2\pi e^\sigma}{\epsilon_a r_{\pm}} e^{\frac{q_{ij}^2}{2\epsilon_a z}} \psi_i(z) \psi_j(z) e^{-\frac{1}{2} q_{ij}^2} \psi_i(z) \psi_j(z) dz \right|^2 \tag{29}
\]
Here, the subindex + refers again to the potential in the region with \( z > 0 \) (and \( r_+ = r \)), while the subindex − to the one with \( z < 0 \) (and \( r_− = 1 \)). The upper and lower signs refer to the regions with \( z > 0 \) and \( z < 0 \), respectively.

In Eqs (28) and (29), \( \Delta \) and \( \Lambda \) are square roughness height and a correlation length.

**Alloy disorder scattering (AD)**

Alloy disorder scattering originates from the randomly varying alloy potential in the barrier. This form of scattering is known [31] to be the mobility-limiting mechanism for 2DEGs confined in an alloy channel such as in heterostructures. In 2DEGs confined in binary wells, alloy scattering occurs as a result of the finite penetration of the 2DEG wavefunction into the barrier. In AlGaN/GaN heterostructures, the large electron effective mass, the high 2DEG density and the large alloy scattering potential all combine to make this form of scattering quite strong in spite of the confinement in the binary semiconductor. With the multisubband, AD scattering can be written [32]:

\[
|V_{ij}^{AD}(q_{ij})|^2 = \int_0^L dz \sum_j \left[ \frac{\{a[x(z)]\}^3 \delta V(x)}{4} x(z) \{1 - x(z)\} \right] \\
\times \left| \sum_{i'j'} \psi_{i'}(z)\psi_{j'}(z) \mathcal{G}^{-1}_{ij,i'j'}(q_{ij}) \right|^2,
\]

where \( a[x(z)] \) and \( \delta V \approx \Delta E_c \) are the lattice constant and alloy scattering potential respectively. Two terms are determined [19]:

\[
a[x(z)] = 3.112 \{x(z)\} + 3.189 \{1 - x(z)\}, \quad x(z) = \frac{z^2}{L^2}
\]

\[
\Delta E_c(x) = 0.63 \{E_g(x) - E_g(0)\},
\]

in which

\[
E_g(x) = 6.28x + 3.42(1 - x) - x(1 - x)
\]

**Screening effect**

The dielectric function \( \varepsilon(q_{ij}) \) in Eqs. (28), (29) and (30) takes account of the screening of scattering potentials by the 2D carriers. As usual, this is evaluated within the random phase approximation [22]:

\[
\varepsilon(q_{ij}) = 1 + \frac{q_s}{q_{ij}} F_{ij,i'j'}(q_{ij}) [1 - G(q_{ij})]
\]

Here, \( q_s = \frac{2m^*e^2}{\varepsilon_0 \hbar^2} \) is the inverse 2D Thomas-Fermi screening length, with \( \varepsilon_0 \) as the dielectric constant of the well layer. The local field corrections due to a many-body exchange effect in the in-plane are quantified by \( G(q_{ij}) = \frac{q_{ij}}{2} \sqrt{\mathcal{F}_i^2 + k_{F_i}k_{F_j}} \mathcal{F}_j \).

\( q_{ij} \) is the 2D momentum transfer due to a scattering event in the in-plane (in polar coordinates): \( q_{ij} = \sqrt{k_{F_i}^2 + k_{F_j}^2 - 2k_{F_i}k_{F_j} \cos \theta} \); with \( \theta \) as a scattering angle, with \( k_{F_i} \) as the Fermi wave number \( k_{F_i} = \sqrt{\frac{2m^*E_{Fi}}{\hbar^2}} \).
The screening form factor $F_{Sij,i'j'}(q_{ij})$ takes account of the extension of particle states along the growth direction.

$$F_{Sij,i'j'}(q_{ij}) = \int_{-\infty}^{+\infty} dz \int_{-\infty}^{+\infty} dz' |\psi(z)|^2 e^{-q(z-z')} |\psi(z')|^2$$  \hspace{1cm} (33)

### 3. Numerical Results

We calculated the multisubband electron mobility between the first and second subband in the semiparabolic quantum wells based on AlN/Al$_x$Ga$_{1-x}$N/AlN. More specifically, we changed the parameters of the material system to investigate the multisubband electron mobility, e.g. dependences of the multisubband electron mobility on alloy content $x$ and the applied electric field $F$.

The physical parameters used in our calculations are chosen as follows [19, 20]: $m_z$(Al$_x$Ga$_{1-x}$N) vs $x$, $m^*$ (Al$_x$Ga$_{1-x}$N) vs $x$.

To estimate the role of the confining potentials effect on the electron confinement in quantum wells, we show the partial confining potentials and the total confining potential for QW width $L = 50\text{Å}$, applied electric field $F = 100 \text{kV/cm}$, and the content of Al in Al$_x$Ga$_{1-x}$N alloy $x = 0.3$ in Figure 2a.

![Figure 2. (a) The partial and total confining potentials. (b) Modul square of the wave function in the lowest two subband.](image)

It can be clearly seen that the polarization induced potential effects the most strong in all of confining potentials. The variation of the semiparabolic confining potential profile by the polarization charges at interface is significantly more the external electric field. The form of the total potential change into the triangle-like at the bottom of quantum well.

In Figure 2b shows modul square of the wave function in the lowest two subband vs the content of Al in Al$_x$Ga$_{1-x}$N alloy $x = 0.3$, $T = 70 \text{ K}$, well width $L = 70 \text{ Å}$ without applied electric field. We can see that the peak of two wave function is different, so it is difficult for intrasubband transition to occur. It means intersubband transition still prevail.
(a) The AD multisubband electron mobility and the PSR multisubband electron mobility.

(b) The AD multisubband electron mobility and the total multisubband electron mobility.

(c) The PSR multisubband electron mobility and the total multisubband electron mobility.

**Figure 3.** The multisubband electron mobility vs the content of Al.

In Figure 3 shows the multisubband electron mobility vs the content of Al in Al\_xGa\_{1-x}N alloy \( x = 0.2-0.5 \), \( T = 70 \) K, \( \Delta = 3 \) Å, \( \Lambda = 50 \) Å, various quantum well widths \( L = 50, 70, \) and 90 Å without applied electric field.

The multisubband electron mobility vs applied electric field (\( F = 0 \) kV/cm to 150 kV/cm) with the content of Al in Al\_xGa\_{1-x}N alloy \( x = 0.2, 0.3, 0.4; T = 70 \) K; \( \Delta = 3 \) Å; \( \Lambda = 50 \) Å; well widths \( L = 70 \) Å is plotted in Figure 4.

From obtained results in Figure 2, 3 and 4, we may draw the following conclusions.

i) Both alloy disorder scattering and interface roughness scattering effect on the multisubband electron mobility but interface roughness scattering is a key scattering. It means that the multisubband electron mobility is changed mainly by the content of Al in Al\_xGa\_{1-x}N alloy. Since the density of polarization charges \( \sigma \) is a function of \( x \) following \( \sigma (x) = 3.075x^2 + 3.70625x \) (|e|)/cm\(^2\). Moreover, changing of the content of Al will give different the height barriers \( V_0 \) and
Figure 4. The multisubband electron mobility corresponding to different values $F$.

(a) The AD multisubband electron mobility and the PSR multisubband electron mobility. (b) The AD multisubband electron mobility and the total multisubband electron mobility.

(c) The PSR multisubband electron mobility and the total multisubband electron mobility.

the area density of electron.

ii) The density of polarization charges will rise when increasing the content of Al to make 2DEG may be drifted to barrier. As a result, the AD multisubband electron mobility, the PSR multisubband electron mobility and the total multisubband electron mobility decrease due to increasing the content of Al.

iii) The external applied electric field has only slightly effect on the multisubband electron mobility. Therefore, the internal structure parameters (polarization, content of Al in Al$_x$Ga$_{1-x}$N alloy, the effective width of the potential well) are more important.

4. Conclusions
To summarize, we have determined that both an external applied electric field and the internal structure parameters have an effect on multisubband mobility but the internal structure
parameters are more important. This results is a basis for next calculations related to transport and optical properties of the semiparabolic quantum wells based on polar materials. Not long ago, part of the application of the work was used to study linear intersubband optical absorption in the semiparabolic quantum wells based on AlN/AlGaN/AlN under a uniform electric field [33].

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