# Electron mobility limited by surface and interface roughness scattering in $Al_xGa_{1-x}N$/GaN quantum wells*

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The electron mobility limited by the interface and surface roughness scatterings of the two-dimensional electron gas in $Al_xGa_{1-x}N$/GaN quantum wells is studied. The newly proposed surface roughness scattering in the AlGaN/GaN quantum wells becomes effective when an electric field exists in the $Al_xGa_{1-x}N$ barrier. For the AlGaN/GaN potential well, the ground subband energy is governed by the spontaneous and the piezoelectric polarization fields which are determined by the barrier and the well thicknesses. The thickness fluctuation of the AlGaN barrier and the GaN well due to the roughnesses cause the local fluctuation of the ground subband energy, which will reduce the 2DEG mobility.

**Keywords:** AlGaN/GaN quantum wells, surface roughness scattering, polarization fields, mobility

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## 1. Introduction

The properties of the III-nitrides and their heterostructures have attracted much research attention over the last decades due to their emerging importance for fabricating short-wavelength emitters and detectors, and due to their inherently superior electronic properties in advanced high power and high temperature applications. The III-nitrides are always heteroepitaxially grown either by metal-organic vapor phase epitaxy (MOVPE)[1–3] or by molecular beam epitaxy (MBE)[4–6] on foreign substrates. The wurtzite structure has a large spontaneous polarization induced by its noncentrosymmetry and a piezoelectric polarization induced by the lattice mismatch between the film and the substrate. It is well known that the two-dimentional electron gas (2DEG) properties of AlGaN/GaN quantum wells (QWs) grown along the $c$(0001) axis are strongly affected by the internal electric field,[7,8] which arises from the spontaneous and piezoelectric polarization discontinuity between the GaN well and the AlGaN barrier. For the $Al_xGa_{1-x}N$/GaN potential well, the ground subband energy is governed by the polarization electric fields which are determined by the barrier and the well thicknesses. In the device fabrication, thin AlGaN/GaN QWs with an abrupt heterointerface are required. In general, the grown heterointerfaces in the AlGaN/GaN QWs are not perfectly smooth on the atomic scale,[9] therefore, both the GaN quantum well and the AlGaN barrier widths show thickness fluctuation of the order of monolayer. For an AlGaN/GaN QW with a thickness of just a few nanometers, the thickness fluctuation will cause the local fluctuation of the polarization field,[10–12] and consequently cause the fluctuation of the ground subband energy, resulting in reduced electron mobility. The scattering induced by the well thickness fluctuation is defined as the interface roughness scattering,[13,14] while the scattering induced by the barrier thickness fluctuation is defined as the surface roughness scattering (see Fig. 1). Liu *et al.* calculated the influence of the barrier thickness fluctuation on the mobility, and they concluded that the mobility decreases as the barrier thickness increases.[15] In this paper, both the interface and the surface roughness scatterings are taken into account to calculate the electron mobility in AlGaN/GaN QWs.

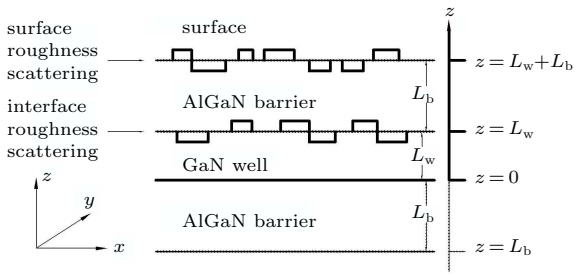



**Fig. 1.** Schematic diagram of the interface and surface roughnesses in AlGaN/GaN QW.

## 2. Calculation

The Hamiltonian of electron in the $Al_xGa_{1-x}N$/GaN potential well is given by

$$H = H_0 + H', \tag{1}$$

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where

$$H_0 = -\frac{\hbar^2}{2m^*}\nabla^2 + V_0 \tag{2}$$

is the main Hamiltonian of the quantum system, with $m^*$ being the electron effective mass,

$$H' = \begin{cases} eF_b z, & \text{for} \quad -L_b \le z \le 0, \\ eF_w z, & \text{for} \quad 0 \le z \le L_w, \\ eF_b(z - L_w - L_b), & \text{for} \quad L_w \le z \le L_w + L_b, \end{cases} \tag{3}$$

describes the perturbation of the polarization field-dressed well and barrier. The quantization direction is along the $z$ axis (see Fig. 1). The $F_w$ and $F_b$ are the polarization fields in the well and the barrier layers of the $Al_xGa_{1-x}N$/GaN QWs, respectively. And

$$V_0 = \begin{cases} \Delta E_C, & \text{for} \quad -L_b \le z < 0, \\ 0, & \text{for} \quad 0 \le z < L_w, \\ \Delta E_C, & \text{for} \quad L_w \le z \le L_w + L_b, \end{cases} \tag{4}$$

where $\Delta E_C = 0.7\Delta E_g$, $\Delta E_g$ is the energy gap difference of the AlGaN barrier and the GaN well, which can be expressed as $\Delta E_g = E_g(Al_xGa_{1-x}N) - E_g(GaN)$, and $E_g(Al_xGa_{1-x}N) = 6.28x + 3.50(1-x) - bx(1-x)$, with $b = 1.3$ eV.

For (0001)-oriented $Al_xGa_{1-x}N$/GaN QWs, the total polarization $P$ is the sum of the spontaneous polarization $P_{sp}$ and the piezoelectric polarization $P_{pz}$, i.e., $P = P_{sp} + P_{pz}$.[16] The electric fields $F_w$ and $F_b$ depending on well thickness $L_w$ and barrier thickness $L_b$ read[17–19]

$$F_w = \frac{(P_b - P_w)L_b}{\varepsilon_b L_w + \varepsilon_w L_b}, \quad F_b = \frac{(P_w - P_b)L_w}{\varepsilon_b L_w + \varepsilon_w L_b}, \tag{5}$$

where $\varepsilon_w(\varepsilon_b)$ is the dielectric constant of the well (barrier).

First, we solve the Schrödinger and the Poisson equations of the $Al_xGa_{1-x}N$/GaN QW self-consistently, and an exact electron wave function and the confined potential profile of the $Al_xGa_{1-x}N$/GaN QW are obtained as shown in Fig. 2.

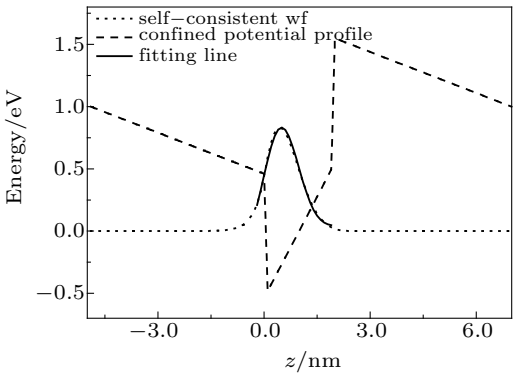



**Fig. 2.** (color online) Ground electron wave function (dotted line) and confined potential profile (dashed line) of an $Al_xGa_{1-x}N$/GaN QW obtained by solving the Schrödinger and the Poisson equations self-consistently, the solid line is the fitting wave function.

Then, the analytical function

$$\psi_1(z) = c\exp(b(z+a))\sin(z+a) \tag{6}$$

is used to fit the wave function (wf) obtained from the self-consistent method, and the fitting function (the blue line) is also presented in Fig. 2. Here, $a, b$, and $c$ are the fitting parameters. We find that there is almost no difference between the two wave functions, so $\psi_1(z)$ can be used for latter calculation.

According to the perturbation theory, the ground subband energy $E_1$ in the $Al_xGa_{1-x}N$/GaN QW is given by

$$E_1 = E_1^0 + \langle\psi_1|H'|\psi_1\rangle, \tag{7}$$

where $E_1^0$ is the ground subband energy in the finite $Al_xGa_{1-x}N$/GaN square well.

A change in well width $\Delta_w(r)$ or barrier width $\Delta_b(r)$ in an atomic scale will cause a local fluctuation $\delta E_1$ in the ground subband energy. Such energy fluctuation can be separated into two parts. One stemming from the interface roughness is denoted as $\delta E_{int}$, and the other stemming from the surface roughness is denoted as $\delta E_{sur}$. The total $\delta E_1$ then reads

$$\delta E_1 = \delta E_{int} + \delta E_{sur}, \tag{8}$$

where

$$\delta E_{int} = \left(\frac{\partial E_1}{\partial L_w}\right)\Delta_w(r) = \left(\frac{\partial E_1}{\partial F_w}\frac{\partial F_w}{\partial L_w} + \frac{\partial E_1}{\partial F_b}\frac{\partial F_b}{\partial L_w}\right)\Delta_w(r), \tag{9}$$

$$\delta E_{sur} = \left(\frac{\partial E_1}{\partial L_b}\right)\Delta_b(r) = \left(\frac{\partial E_1}{\partial F_w}\frac{\partial F_w}{\partial L_b} + \frac{\partial E_1}{\partial F_b}\frac{\partial F_b}{\partial L_b}\right)\Delta_b(r). \tag{10}$$

It is assumed that the roughnesses $\Delta_w(r)$ and $\Delta_b(r)$ oriented along the $z$ axis follow the same Gaussian distribution, and we assume $\Delta_w = \Delta_b = \Delta$, $\Lambda_w = \Lambda_b = \Lambda$ here for simplicity. Then, the interface and surface roughness can be expressed with the Gaussian autocorrelation function[20]

$$\langle\Delta(r)\Delta(r')\rangle = \Delta^2\exp\left(-\frac{|r-r'|^2}{\Lambda^2}\right), \tag{11}$$

where $\langle\cdots\rangle$ means an ensemble average. Using the Fourier series for the right-hand side of Eq. (11), the square of two-dimensional scattering matrix element $|M_R|^2$ can be expressed as

$$|M_R|^2 = \pi\Delta^2\Lambda^2|\delta E_1|^2\exp\left(-\frac{q^2\Lambda^2}{4}\right). \tag{12}$$

The scattering rate $1/\tau_R(E)$ due to interface and surface roughness scatterings is then given by

$$\frac{1}{\tau_R(E)} = \left(\frac{2\pi}{\hbar}\right)\frac{1}{(2\pi)^2}\int|M_R|^2 S_C(1-\cos\theta) \times\delta(E_{k'} - E_k)\,\mathrm{d}^2k', \tag{13}$$

where $S_C = \left[q/(q+q_{TF})\right]^2$ is the screening factor with $q_{TF} = 2/a_B^*$ being the Thomas–Fermi wave vector, and $a_B^* = 4\pi\hbar^2\varepsilon/(m^*e^2)$ is the effective Bohr radius in the quasi-2DEG of GaN. The electron mobility in AlGaN/GaN QWs can be expressed as $\mu = e\tau_R(E)/m^*$.

## 3. Results and discussion

Now we give the calculated results of the 2DEG mobility. In this paper, the electron effective mass is $m_e^* = 0.22m_0$. The height $\Delta = 2.59$ Å corresponds to the thickness of one monolayer GaN.

To describe the interface and surface roughness, there are two variables, roughness height $\Delta$ and lateral size $\Lambda$, representing the roughness. The mobility versus roughness lateral size $\Lambda$ for different roughness height $\Delta$ is shown in Fig. 3. The mobility first decreases with increasing roughness lateral size $\Lambda$, and then increases across a minimum value, because $\Lambda$ is a two-value function of mobility from Eq. (12). Apparently, there are two $\Lambda$ values for the same mobility and a given $\Delta$. And it is also seen that the mobility increases sharply with decreasing roughness height $\Delta$, which shows that the height $\Delta$ should be smaller for obtaining a large mobility.

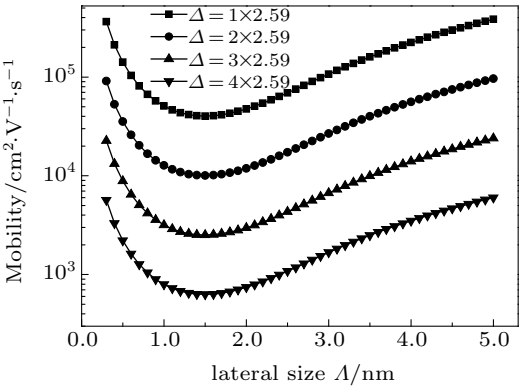



**Fig. 3.** Variation of mobility with the roughness lateral size $\Lambda$ for different roughness height $\Delta$. Here, well width $L_w = 2$ nm and barrier width $L_b = 5$ nm are adopted.

Figure 4 shows the sheet carrier density dependence of the mobility limited by the surface and interface roughness scatterings for different lateral size $\Lambda$. As a result of the interface and surface roughness scatterings, the mobility increases monotonically as the sheet carrier density increases from $1 \times 10^{12}$ cm$^{-2}$ to $1 \times 10^{13}$ cm$^{-2}$. Because the 2DEG density $N_s$ increases with widening barrier thickness $L_b$, thus the relation between the mobility and $L_b$ is also set up, which is shown in Fig. 5(a).

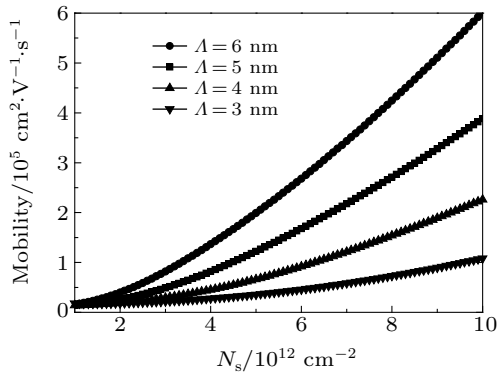



**Fig. 4.** Variation of mobility with the 2DEG density. Here, well width $L_w = 2$ nm, barrier width $L_b = 5$ nm, and roughness height $\Delta = 0.259$ nm are adopted.

The calculated mobility variation as a function of well thickness $L_w$ for several typical barrier thicknesses $L_b$ is presented in Fig. 5(a), and the mobility as a function of barrier width $L_b$ for several typical $L_w$ is plotted in Fig. 5(b). As shown in Fig. 5, with increasing $L_b$ or $L_w$ the mobility increases monotonically. That is, with the same roughness variables $\Delta$ and $\Lambda$, increasing $L_b$ or $L_w$ is an effective way to increase the mobility. The same thickness fluctuation $\Delta(r)$ will cause more serious inhomogeneity of the polarization field in the thinner barrier or well than that in the thicker ones, because the ratio of $\Delta(r)/L_b$ or $\Delta(r)/L_w$ is higher for smaller $L_b$ or $L_w$. Thongnum has reported that with the same $\Delta$, the fluctuation potential decreases with increasing $L_w$.[13] In our work, with increasing $L_w$ or $L_b$, the potential fluctuation decreases, which means smaller roughness scattering and larger mobility. It can also be observed that the dependences of mobility on $L_b$ (Fig. 5(b)) are similar to those on $L_w$ (Fig. 5(a)), the only difference is that the former changes more gently than the latter, which demonstrates that $L_w$ has a more prominent influence on the 2DEG mobility than $L_b$. It can be explained by that the electrons mostly confined in the quantum well are more sensitive to the fluctuation of well width $L_w$ than that of barrier width $L_b$ when $L_b$ is not so small.

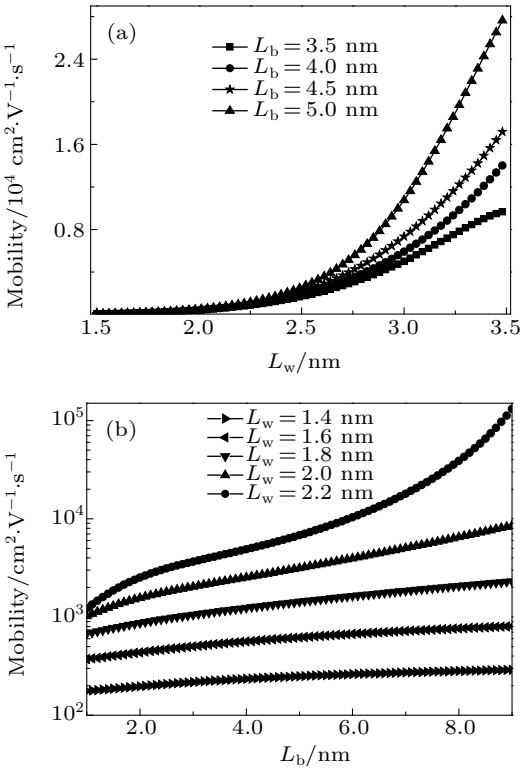



**Fig. 5.** (a) Variation of mobility with well width $L_w$ for different $L_b$; (b) variation of mobility with barrier width $L_b$ for different $L_w$. Here, roughness height $\Delta = 0.259$ nm, lateral size $\Lambda = 5$ nm, $N_s = 1 \times 10^{13}$ cm$^{-2}$ are adopted.

The calculated mobility variation as a function of well thickness $L_w$ and barrier width $L_b$ for different Al molar fraction ($x = 0.3, 0.6$) is shown in Fig. 6. It can be easily seen that the mobility for $x = 0.6$ is larger than that for $x = 0.3$. The mobility increases as the Al molar fraction increases. AlGaN with a low Al molar fraction (such as $x = 0.2$–$0.3$) is

always adopted for current AlGaN/GaN devices, which is because that the growth of AlGaN with a high Al molar fraction is very difficult. The AlGaN films and heterostructures with a high Al molar fraction will be extensive used once the growth problems are conquered.

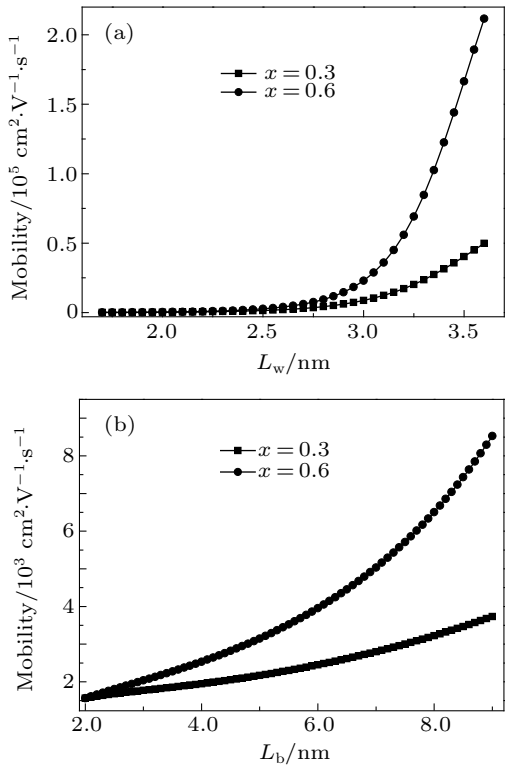



**Fig. 6.** Variations of mobility with (a) well width $L_w$ and (b) barrier width $L_b$ for different Al molar fraction in AlGaN barrier layer. Here, roughness height $\Delta = 0.259$ nm, lateral size $\Lambda = 5$ nm, $N_s = 1 \times 10^{13}$ cm$^{-2}$ are adopted.

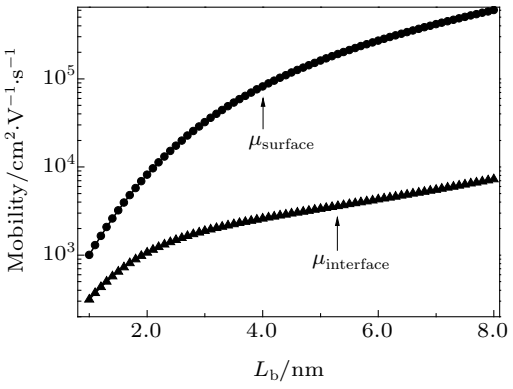



**Fig. 7.** Barrier width $L_b$ dependence of surface and interface roughness scatterings. Here, the parameters are chosen to be $L_w = 2.2$ nm, $\Delta = 0.259$ nm, $\Lambda = 5$ nm, $N_s = 1 \times 10^{13}$ cm$^{-2}$.

The mobilities varying with the interface roughness scattering ($\mu_{interface}$) and the surface roughness scattering ($\mu_{surface}$) are shown in Fig. 7. The $\mu_{interface}$ and $\mu_{surface}$ both increase as $L_b$ increases, because the two scatterings both become weaker with increasing barrier width $L_b$. It is also clearly seen that $\mu_{surface}$ is larger than $\mu_{interface}$ at arbitrary barrier width $L_b$, which indicates that the interface roughness scattering is still stronger than the surface roughness scattering. However the surface roughness scattering still plays an important role in decreasing the mobility, which must also be considered.

## 4. Conclusion

In summary, we investigated the 2DEG mobility limited by the familiar interface roughness scattering and a newly proposed surface roughness scattering in $Al_xGa_{1-x}N$/GaN QWs. It is found that the mobility increases with increasing well width $L_w$ or barrier width $L_b$, which shows that the mobility can be modulated by the widths of the barrier and the well under the same roughness variables. And the interface roughness scattering is found to be stronger than the surface roughness scattering under the same condition. However the surface roughness scattering still plays an important role in decreasing the mobility, which cannot be ignored compared to the interface roughness scattering.

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