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The mobility of two-dimensional electron gas in AlGaN/GaN heterostructures with varied Al content

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The mobility of the two-dimensional electron gas (2DEG) in AlGaN/GaN heterostructures changes significantly with Al content in the AlGaN barrier layer, while few mechanism analyses focus on it. Theoretical calculation and analysis of the 2DEG mobility in AlGaN/GaN heterostructures with varied Al content are carried out based on the recently reported experimental data. The 2DEG mobility is modeled analytically as the total effects of the scattering mechanisms including acoustic deformation-potential, piezoelectric, polar optic phonon, alloy disorder, interface roughness, dislocation and remote modulation doping scattering. We show that the increase of the 2DEG density, caused by the ascension of the Al content in the barrier layer, is a dominant factor that leads to the changes of the individual scattering processes. The change of the 2DEG mobility with Al content are mainly determined by the interface roughness scattering and the alloy disorder scattering at 77 K, and the polar optic phonon scattering and the interface roughness scattering at the room temperature. The calculated function of the interface roughness parameters on the Al content shows that the stress caused AlGaN/GaN interface degradation at higher Al content is an important factor in the limitation of the interface roughness scattering on the 2DEG mobility in AlGaN/GaN heterostructures with high Al content.

GaN, heterostructures, 2DEG, mobility

1 Introduction

The GaN HEMT devices have shown widely the superior performance in the high frequency, high voltage and large power applications. The core AlGaN/GaN heterostructures as shown in

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Figure 1 feature excellent electric conductivity that is supplied by the quantized two-dimensional electron gas (2DEG). The great amount of experimental data published[1−8] show that the Al content in the AlGaN barrier layer of AlGaN/GaN heterostructures has a strong impact on the 2DEG density and mobility. The mechanism of such a phenomenon is an important guideline in the optimization of GaN-based heterostructures for electronic devices.

The almost linearly increase of 2DEG density with Al content has been widely ascribed to the strong polarization effects of the III-N compounds and can be modeled precisely[1−3]. While the Al content dependent 2DEG mobility has very few theoretical explanation. A quantitative calculation was presented by Miyoshi et al.[8], but the brief analysis focused only on the interface roughness scattering and the dislocation scattering, and some other involved scattering processes are dealt with improperly.

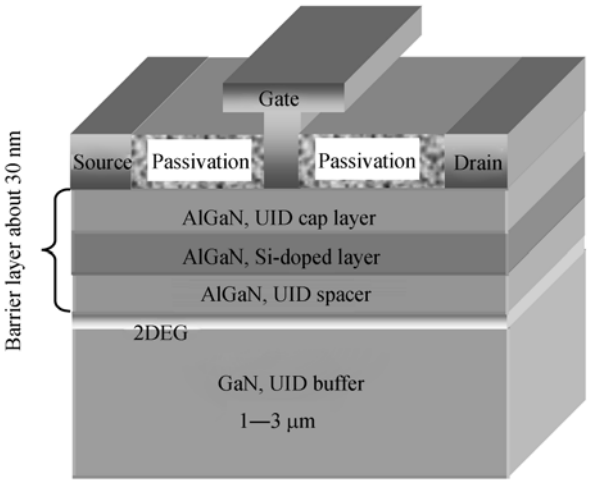

Figure 1 Typical AlGaN/GaN HEMT structures.

In this paper, we present a theoretical investigation on the 2DEG mobility of AlGaN/GaN heterostructures with varied Al content at 77 K and room temperature (RT). The 2DEG mobility is modeled analytically as the total effects of various scattering mechanisms. The internal mechanisms of the Al content dependence of the 2DEG mobility are revealed through the detailed analysis of all the scattering processes. The mobility data reported by Miyoshi et al. are used as the experimental proof of our calculation, and the problems present in their theoretical analysis are also pointed out.

2 Model

According to the Matheissen's rule, the 2DEG mobility is related to the mobilities of various scattering mechanisms as follows:

$$\mu^{-1} = \sum_i \mu_i^{-1}. \tag{1}$$

The component mobility μ_i satisfies $\mu_i = e\tau_i / m^*$ in the momentum relaxation approximation, where τ_i is the momentum relaxation time, and m^* is the electron effective mass. The density of 2DEG in nitride heterostructures is generally quite high, so the scattering mechanisms considered

including acoustic deformation-potential, piezoelectric, polar optic phonon, alloy disorder, interface roughness, dislocation and remote modulation doping scattering are all formulized based on the 2D degenerate statistics of 2DEG. The exact Hartree-Fork wave function is approximated by the analytical Fang-Howard variational wave function for simplicity[9], so the wave function distribution is determined once the 2DEG density is given. The analytical expressions of the momentum relaxation rates $1/\tau_i$ for the scattering mechanisms are briefly summarized below and the related material parameters are listed in Table 1.

Table 1 The related material parameters used in the mobility calculation

Electron effective mass of GaN and AlGaN	$m^* = 0.20\ m_0$, $m_x^* = (0.2 + 0.2\ x)\ m_0$[16]
Deformation potential	$a_C = 9.10$ eV[17]
Mass density	$\rho = 6.15$ g • cm^{-3}[16]
Longitudinal acoustic phonon velocity	$v_s = 8.00 \times 10^5$ cm·s^{-1}[16]
Static and high frequency dielectric constant	$\varepsilon_s = 8.90$, $\varepsilon_h = 5.35$[16]
Electromechanical coupling coefficient	$M^2 = 0.039$ [11]
Polar optic phonon energy	$\hbar\omega_{\mathrm{POL}} = 91.2$ meV[16]
Lattice constant of AlGaN	$a_0(x) = (0.3189 + 0.0077\ x)$ nm[16] $c_0(x) = (0.5186 + 0.0204\ x)$ nm[16]
Alloy scattering potential of AlGaN	$V_A - V_B = 1.80$ eV[18]
Conduction band offset	$\Delta E_C(x) = 0.75(E_{g(\mathrm{AlGaN})} - E_{g(\mathrm{GaN})})$[1]
Thomas-Fermi wavevector	$q_{\mathrm{TF}} = 8.4994 \times 10^8$ m^{-1}
Dislocation filling factor	$f_{\mathrm{DIS}} = 0.3$[19]

The acoustic deformation-potential (DP) scattering is expressed as[10]

$$\frac{1}{\tau_{\mathrm{DP}}} = \frac{3m^* {a_C}^2 k_B T}{16\rho {v_s}^2 \hbar^3} b, \tag{2}$$

where $b = (\dfrac{33m^* e^2 n_{s2D}}{8\hbar^2 \varepsilon_0 \varepsilon_s})^{1/3}$ is a variational parameter, and n_{s2D} is the 2DEG sheet density.

The piezoelectric (PE) scattering is expressed as [11]

$$\frac{1}{\tau_{\mathrm{PE}}} = \frac{e^2 M^2 k_B T m^*}{4\pi\varepsilon_0 \varepsilon_s \hbar^3 {k_{\mathrm{F}}}^3} \int_0^{2k_F} \frac{F(q) q^3}{(q + q_{\mathrm{TF}} F(q))^2 \sqrt{1 - (q/(2k_{\mathrm{F}}))^2}} dq, \tag{3}$$

where $k_{\mathrm{F}} = \sqrt{2\pi n_{s2D}}$ is the Fermi wave vector, and $q = 2k_F \sin(\theta/2)\ \theta \in (0, \pi)$ is the difference of the wave vectors between the initial state and the final state in scattering. The quantity $q_{\mathrm{TF}} = m^* e^2/(2\pi\varepsilon_0 \varepsilon_s \hbar^2)$ is the Thomas-Fermi wave vector and reflects the screening length of 2DEG, and $F(q) = \eta^3$ and $G(q) = (2\eta^3 + 3\eta^2 + 3\eta)/8$ with $\eta = b/(b+q)$ are two-form factors out of the Fang-Howard wave function. The quantity $G(q)$ presents below in eqs. (4), (6) and (8).

The polar optic phonon (POL) scattering is expressed as [12]

$$\frac{1}{\tau_{\mathrm{POL}}} = \frac{e^2 \omega_{POL} m^* N_B(T) G(k_o)}{2\varepsilon^* k_o \hbar^2 P_{\mathrm{POL}}(y)}, \tag{4}$$

where there is $\varepsilon^* = \varepsilon_0/(1/\varepsilon_h - 1/\varepsilon_s)$. The quantities $\hbar\omega_{\mathrm{POL}}$ and $k_o = \sqrt{2m^*(\hbar\omega_{\mathrm{POL}})/\hbar^2}$ are the energy and the wave vector of the polar optic phonon respectively, $N_{\mathrm{B}}(T) = \dfrac{1}{\exp(\hbar\omega_{\mathrm{POL}}/k_{\mathrm{B}}T) - 1}$

is the Bose-Einstein distribution function, and $P_{\mathrm{POL}}(y) = 1 + (1 - e^{-y})/y$ is with a dimensionless variable $y = \pi\hbar^2 n_{s2D} / (m^* k_{\mathrm{B}} T)$.

The alloy disorder (ADO) scattering is expressed as [13]

$$\frac{1}{\tau_{\mathrm{ADO}}} = \frac{m^* \Omega(x)(V_A - V_B)^2 x(1-x)}{\hbar^3} \int_{-\infty}^{0} \psi^4(z)\, dz, \tag{5}$$

where $\Omega(x) = (\sqrt{3}/2) c_0(x) \cdot a_0{}^2(x)$ is the volume of the unit cell of the wurtzite AlGaN, and $\psi(z)$ is the modified Fang-Howard wave function.

The interface roughness (IFR) scattering is expressed as[14]

$$\frac{1}{\tau_{\mathrm{IFR}}} = \frac{\Delta^2 L^2 e^4 m^*}{2(\varepsilon_0 \varepsilon_s)^2 \hbar^3} \left(\frac{1}{2} n_{s2D} \right)^2 \int_0^1 \frac{u^4 \exp(-k_{\mathrm{F}}{}^2 L^2 u^2)}{[u + G(q) q_{\mathrm{TF}}/(2k_{\mathrm{F}})]^2 \sqrt{1-u^2}}\, du, \tag{6}$$

where Δ is the root mean square (RMS) roughness, and L is the correlation length. Usually they are combined to show the interface roughness.

The dislocation (DIS) scattering is expressed as [15]

$$\frac{1}{\tau_{\mathrm{DIS}}} = \frac{N_{\mathrm{DIS}} m^* e^4 f_{\mathrm{DIS}}{}^2}{\hbar^3 \varepsilon_0^2 \varepsilon_s^2 c_0^2(0)} \cdot \frac{1}{4\pi k_{\mathrm{F}}^4} \int_0^1 \frac{du}{[u + q_{\mathrm{TF}}/(2k_{\mathrm{F}})]^2 \sqrt{1-u^2}}, \tag{7}$$

where N_{DIS} is the 2D density of threading edge dislocations, f_{DIS} is the occupancy of the states in the energy band gap introduced by the dislocations and $u = q/(2k_F)$ is used for simplicity.

The remote modulation doping (MD) scattering is expressed as [10]

$$\frac{1}{\tau_{\mathrm{MD}}} = N_{\mathrm{D}} \frac{m^*}{4\pi\hbar^3 k_{\mathrm{F}}^3} \left(\frac{e^2}{2\varepsilon_0 \varepsilon_s} \right)^2 \int_0^{2k_{\mathrm{F}}} \frac{F(q)^2 [\exp(-2qd_2) - \exp(-2qd_1)] q}{[q + q_{\mathrm{TF}} G(q)]^2 \sqrt{1 - (q/(2k_{\mathrm{F}}))^2}}\, dq, \tag{8}$$

where N_{D} is the doping density and the distances between the boundaries of the modulation doped part and the AlGaN/GaN heterointerface are d_1 and d_2 with $d_1 > d_2$.

3 Results and discussion

The AlGaN/GaN heterostructures reported by Miyoshi et al.[8] are grown by metal organic chemical vapor deposition (MOCVD) on sapphire. The AlGaN barrier layer consists of, from top to bottom, a 3-nm-thick undoped layer, a 15-nm-thick silicon-doped layer with a doping density of $N_{\mathrm{D}} = 5\times10^{18}$ cm^{-3}, a 7-nm-thick undoped layer (d_1 = 22 nm and d_2 = 7 nm). The dislocation density is $N_{\mathrm{DIS}} = 3\times10^9$ cm^{-2} for GaN layer. The nominal values are adopted for these parameters in the calculation. The Hall data for these structures include the 2DEG density and mobility at 77 K and RT. When the Al content x increases from 0.16 to 0.42, the 2DEG density n_{s2D} at 77 K increases almost linearly from about 7×10^{12} cm^{-2} to about 1.7×10^{13} cm^{-2}, and the curve moves a little upward at RT. The 2DEG mobility at 77 K decreases from about 6600 to about 2000 cm^{2}V^{-1}s^{-1}, and the 2DEG mobility at RT decreases from about 1400 to about 900 cm^{2}V^{-1}s^{-1}.

In the mobility calculation, the measured n_{s2D}—x curve at 77 K is linearly fitted and used to calculate the mobility of each scattering mechanism. To allow for the possibility of the x dependent AlGaN/GaN interface roughness, the IFR scattering mobility is deduced from eq. (1) within which the measured 2DEG mobility and the total mobility limited by the other scattering mechanisms are substituted. The deduced IFR scattering mobilities at 77 K and RT are very close based

on the above model and parameter settings, and their average value is taken as the calculated IFR scattering mobility. Then the interface roughness parameters are determined.

The relations between the calculated component mobilities of the individual scattering processes with the measured and the calculated 2DEG mobility data are shown in Figure 2. The scattering processes at 77 K, if listed from strong to weak, are IFR, ADO, DP, PE, DIS, and MD scattering, and the mobility of the weakest POL scattering is on the order of 10^7 $cm^2V^{-1}s^{-1}$ and not shown in Figure 2(a). So the decrease of 2DEG mobility at 77 K with x is mainly determined by the IFR and ADO scattering, and especially the IFR scattering is dominant at high x. The other scattering processes show their effect at low x.

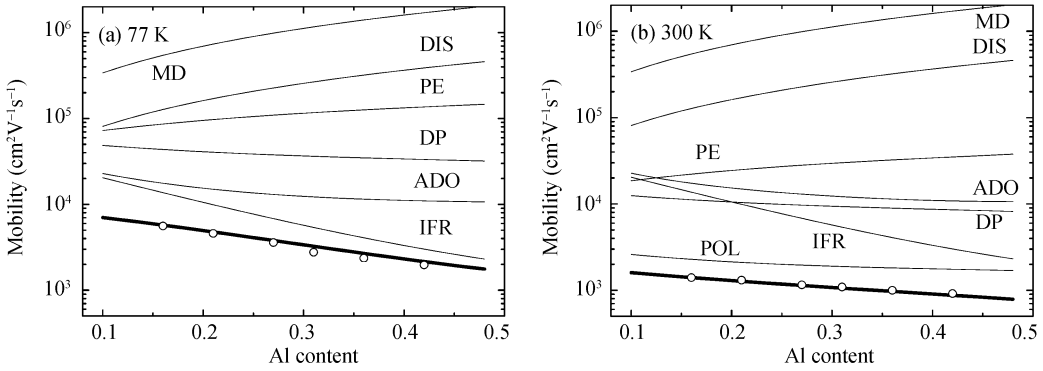

Figure 2 The measured 2DEG mobility and the calculated 2DEG mobility and component mobilities of the individual scattering processes as a function of the Al content x in the AlGaN barrier layer at (a) 77 K and (b) RT. —, Calculated 2DEG mobility; ○, measured 2DEG mobility.

The lattice vibration related DP, PE, and POL scattering are significantly strengthened while the other scattering processes unchanged at RT, and especially the POL scattering becomes the strongest scattering process. It is because when temperature rises, the lattice vibration gets stronger, so does the scattering effect on electrons. In fact the DP and the PE scattering mobilities are proportional to T^{-1}, and the POL scattering mobility decreases exponentially with temperature. The large polar optic phonon energy of GaN (91.2 meV) strengthens the POL scattering further. So the decrease of 2DEG mobility at RT with x is mainly determined by the POL and IFR scattering. The POL scattering dominates in the considered x range, and the IFR scattering is also important at high x.

The mobility of every scattering process changes with the Al content at given temperature. But none of the scattering mechanisms except the ADO scattering are relevant to x according to their momentum relaxation rate models. So the changes of the scattering processes are caused by an increase in n_{s2D}, as a result of polarization effect when the Al content in the AlGaN/GaN structure increases.

The MD scattering is a kind of coulombic scattering, and the scattering center is the ionized donor with the spacer layer between it and the 2DEG. When the donor density N_D is constant and n_{s2D} increases, the screening effect of the electrons on the columbic force is stronger and the scattering effect is weaker, so the mobility increases. The DIS scattering is also Columbic and the scattering center is the charged dislocation lines composed of the suspended bonds, and the line charge density is $e f_{DIS}/c_0(0)$, so the DIS scattering mobility also increases with n_{s2D}. According to

the calculation of Leung et al.[19], when the dislocation density is in the range of $N_{DIS} = 10^8$—10^{10} cm^{-2}, only 10%—50% of the energy states will be occupied ($f_{DIS} = 0.1$—0.5), so $f_{DIS} = 0.3$ is adopted in the calculation. In some undoped AlGaN/GaN structures with low Al content, it is observed that the low temperature 2DEG mobility increases with Al content[20]. The DIS scattering may be one of the principal factors underlying the phenomena.

The DP scattering mobility is proportional to $n_{s2D}^{-1/3}$, so it decreases with n_{s2D}. The PE scattering mobility is a complicated function of n_{s2D}[11], and it increases in the involved n_{s2D} range. The POL scattering mobility decreases almost exponentially with n_{s2D}.

The ADO scattering is directly related to both x and n_{s2D}. The mobility curve based on n_{s2D}—x fitted curve is extended to $x = 0.04$—0.96 for the convenience of discussion and shown in Figure 3. This kind of scattering in AlGaN/GaN structures originates from the effect of the randomly fluctuating Al and Ga atom potential in the AlGaN material on the penetration part of the 2DEG wave function into the barrier layer. When n_{s2D} is higher, the 2DEG penetration is strengthened and the scattering is stronger. When x is higher, on the one hand the alloy disorder extent in AlGaN (proportional to $x(1–x)$) changes, and on the other hand, the energy barrier height at the AlGaN/GaN heterointerface changes. The alloy atom distribution reaches the full disorder extent at $x = 0.5$, and gets more ordered when x deviates from this point. The energy barrier at the AlGaN/GaN interface increases with x. So in the AlGaN/GaN heterostructures with increasing x while constant n_{s2D}, when x is less than 0.5, the scattering is strengthened only at small x because of the more disordered III-group atom distribution, but weakened when x is larger as a result of the weaker 2DEG penetration caused by the higher energy barrier at heterointerface. While x is more than 0.5, both the even weaker 2DEG penetration and the less disordered alloy atom distribution weaken the scattering further. As for the AlGaN/GaN heterostructures with the 2DEG naturally changes its density with x, the ADO scattering mobility reflects the interplay of the above mechanisms, and the dominant factor changes from the increase of n_{s2D} to that of x at the bottom of the mobility curve.

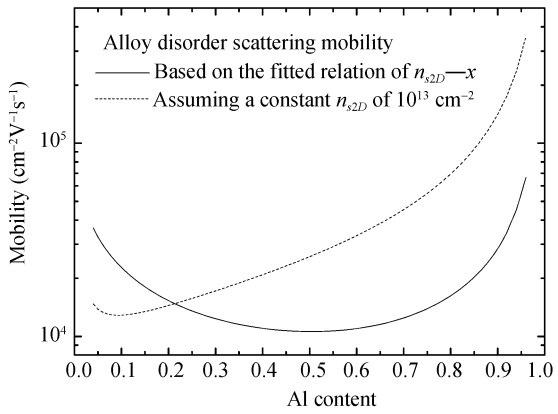

Figure 3 The alloy disorder scattering mobility versus Al content x.

The IFR scattering is very sensitive to n_{s2D}. The heterointerface is a region where the material and lattice atom distribution change irregularly, so the heterointerface is rough and scatters the electrons which transport along the interface. When n_{s2D} increases, the 2DEG electron distribu-

tion shifts closer to the AlGaN/GaN heterointerface and the electron transport becomes more sensitive to the interface roughness, the IFR scattering is stronger and the mobility is lower. The rapid change of the IFR scattering mobility with x in Figure 2 also hints the increased AlGaN/GaN interface roughness. When the Al content of AlGaN/GaN structure increases, the stress in the AlGaN layer is larger, and the surface becomes rougher, as has been confirmed by the atomic force microscopic pictures of the surface morphology of the samples[4,8]. So it is necessary to deduce the RMS roughness Δ and the correlation length L from the IFR scattering mobility and to check whether the interface roughness changes.

But it should be noted that, there is uncertainty in the solution of Δ and L values. As shown in Figure 4, the L dependent IFR scattering mobility curve at given n_{s2D} and Δ has a minimum point, and the curve moves downward when Δ increases. So an infinite series of Δ and L values can be solved for the known IFR scattering mobility and n_{s2D}. For simplicity, we choose Δ with the minimum mobility of the corresponding mobility curve equal to the given mobility as denoted by the Γ point, and then determine a unique pair of Δ and L values. The Δ is the smallest one in all the possible Δ values, so it has a physical meaning of the highest scattering efficiency.

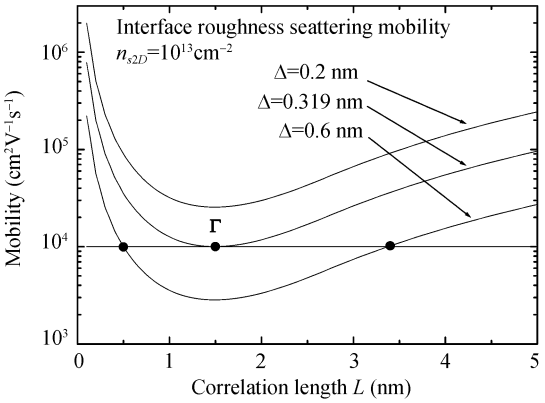

Figure 4 The interface roughness scattering mobility at different RMS roughness Δ as a function of the correlation length L at the 2DEG electron density of 10^{13} cm^{-2}. The solid dots show the possible solutions of Δ and L values for a given mobility of 10^4 cm^{2}V^{-1}s^{-1}.

The x dependent Δ and L determined in the above way are shown in Figure 5. The interface roughness Δ is a little lower and less increased than the observed surface roughness. The difference can be well explained by the stress transfer in the growth of AlGaN barrier layer on GaN layer. In the initial stage, the lattice mismatch caused stress leads to some defects such as misfit dislocations, and the resulting interface roughness increases with x. Usually the AlGaN layer in AlGaN/GaN is only 20 to 30 nm thick, and it is a flexible layer relative to the GaN layer below generally with a thickness of several μm. The growth is from bottom to top, which ensures that the stress transfers upward. So the surface roughness should be higher than the AlGaN/GaN interface roughness, and at higher x the stress increases and surface degradation should be greater than interface degradation. The L in Figure 5 decreases almost linearly with x, suggesting that the points on the interface with structure fluctuation become denser. This accords with the tendency of the increasing interface roughness. In addition, the solved values of Δ and L agree well with the widely adopted empirical values $\Delta \approx 0.3$ nm, $L=1.0-3.0$ nm[21−23] for MOCVD AlGaN/GaN

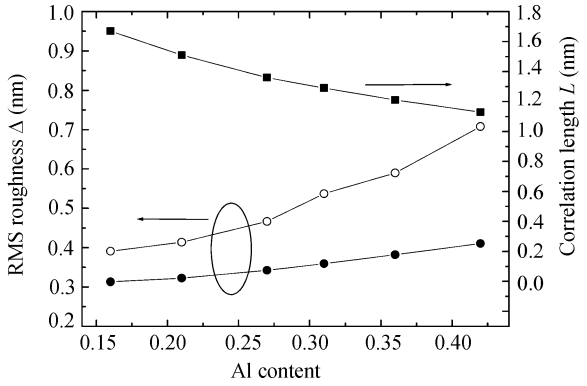

Figure 5 The calculated interface roughness parameters Δ and L as a function of the Al content x for the interface roughness scattering mobility in Figure 2. The measured surface roughness is from ref. [8]. ○, Measured Δ at AlGaN surface; ●, calculated Δ at AlGaN interface; ■, calculated L.

samples, which also shows that the solution is reasonable. The calculation effort of Δ at different values of constant L shows that Δ always changes with x. So increase in the Al content in the AlGaN/GaN structure does degrade the interface. A comparison of such effect with that of n_{s2D} increase on the IFR scattering mobility shows that the latter is more important.

Miyoshi et al. calculated the relation between the various scattering mechanisms and the 2DEG mobility with the theoretical model similar to that of ours, and the scattering mechanisms considered, if the remote modulation doping scattering is added, are the same to that of ours. Their intention is to show that the AlGaN/GaN interface gets rougher at higher Al content, and the interface roughness scattering is an important mechanism to suppress the 2DEG mobility in high Al content heterostructure samples. In our opinion, their basic conclusion is right. But there are several obvious unreasonable points in their theory according to their calculated component mobilities of the individual scattering processes as a function of Al content[8]. First, the mobilities of acoustic deformation-potential scattering and polar optic phonon scattering are independent of Al content. It means that the relation between the two mechanisms and 2DEG density is ignored, but for the other mechanisms the dependence on 2DEG density is taken into consideration, so the model is not self-consistent as a whole. Such a point is quite unreasonable since the two mechanisms are quite important, especially the polar optic phonon scattering at room temperature. Second, the alloy disorder scattering mobility rises with Al content. But the alloy disorder scattering gets stronger at higher Al content in the considered range, and the mobility should fall, as is evident from the analysis of the related physical mechanisms. In addition, the deduction of Δ under the assumption that L is a constant (5.0 nm) independent of Al content is unreasonable. The L value is too large to be true, and assuming a constant L is improper for stress-caused interface roughness increase.

It should be noted that the electron effective mass m^* is a very important factor in the 2DEG mobility calculation, and must be chosen properly. If m^* is small, the momentum relaxation time would be longer in the same scattering condition, and the mobility would rise. Otherwise the mobility would fall. The published m^* value for GaN is dispersive ($0.15-0.23\ m_0$)[24], and the m^* value adopted in this paper is determined after many trials. There is a convenient criterion in the trial, i.e., the m^* value is improper if the deduced Al content dependent interface roughness scattering mobility curves at 77 K and room temperature differ significantly. As we know, the inter-

face roughness scattering is independent of temperature.

4 Conclusions

We investigated the 2DEG mobility of AlGaN/GaN heterostructures with varied Al content at 77 K and room temperature with the analytical model of 2DEG mobility as the combined effects of various scattering mechanisms. It is found that the decrease of 2DEG mobility with Al content at 77 K is mainly determined by the interface roughness scattering and the alloy disorder scattering. The decrease of 2DEG mobility with Al content at room temperature is mainly determined by the polar optic phonon scattering and the interface roughness scattering, and the latter is quite important at high Al content. The changes of the scattering processes when the Al content in the AlGaN/GaN structure increases are principally caused by the accompanying 2DEG density increase. The interface roughness parameters deduced from the calculated interface roughness scattering mobility show that the stress caused by the Al content increase in the AlGaN layer renders the AlGaN/GaN interface rougher, and it is an important factor in the suppression of the interface roughness scattering on the 2DEG mobility in high Al content AlGaN/GaN heterostructures.

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