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Ting-Hsiang Hung, Michele Esposto, and Siddharth Rajan

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Interfacial charge effects on electron transport in III-Nitride metal insulator semiconductor transistors

Ting-Hsiang Hung, Michele Esposto, and Siddharth Rajan
Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio 43210, USA

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We report on the calculation of the two dimension electron gas (2DEG) mobility in scaled AlGaN/GaN metal-insulator-semiconductor high-electron-mobility-transistors. We investigate the effect of remote impurity and phonon scattering models on the 2DEG mobility of the dielectric/AlGaN/GaN structure and investigate its variation with dielectric/AlGaN interface charge density, 2DEG concentration, and AlGaN thickness. Remote impurity scattering was found to be the dominant mechanism when the 2DEG density is below \(5 \times 10^{12} \text{ cm}^{-2}\) and dielectric/AlGaN interface charge density is above \(5 \times 10^{12} \text{ cm}^{-2}\). The interfacial charge has significant effect on the mobility as the AlGaN cap layer thickness is scaled down below 5 nm. © 2011 American Institute of Physics. [doi:10.1063/1.3653805]

AlGaN/GaN high electron mobility transistors (HEMTs) are excellent candidates for high power\(^1\) and high frequency\(^3\) applications due to their superior material properties like high bandgap, high electron velocity, and built-in and piezo-electric polarization. However, in order to improve the performance of AlGaN/GaN HEMTs at even higher frequencies, aggressive vertical and lateral scaling is required. As the gate to channel distance is reduced, gate leakage becomes a significant problem, to mitigate which, metal-insulator-semiconductor high electron mobility transistors (MIS-HEMTs) are used.\(^4\)\textendash\textsuperscript{11} In such highly scaled devices, the insulator/AlGaN interface being very close to the 2DEG can affect the mobility. In this work, we have investigated remote impurity scattering to analyze the effect of dielectric/AlGaN interface charges on 2DEG mobility.

In the AlGaAs/GaAs system, it has been shown that strong scattering at low temperature in the 2DEG system arises from defects or ionized charges which are separated from the 2DEG by a spacer.\(^12\) In the Si-based system, the effect of remote charge scattering on electron mobility has been discussed as the gate oxide thickness becomes ultrathin.\(^13\)\textendash\textsuperscript{15} In the doping-free AlGaN/GaN HEMT system, the above effect is not observed since the polarization dipoles that induce a 2DEG do not have as great an effect on mobility.\(^16\)\textendash\textsuperscript{19} In MIS-HEMTs, as the dimensions of devices scale down, the AlGaN layer becomes thinner and the 2DEG experiences increased scattering due to the fixed charge between dielectric and AlGaN layers. Figure 1 shows the schematic energy band diagrams and charge distribution for Ga-polar and N-polar MIS-HEMT structures used for our calculations.

The tensile strain caused by the growth of AlGaN on GaN results in a piezoelectric polarization charge \(\sigma_{PE}\), which adds to the spontaneous polarization charge \(\sigma_{SP}\), and gives positive net polarization charge at the AlGaN/GaN interface; \(\sigma_{PE}\) and \(\sigma_{SP,AlGaN}\) gives negative net polarization charge at the dielectric/AlGaN interface. In the case of Ga-polar structures (Fig. 1(a)), there is a net negative polarization charge at the dielectric/semiconductor interface, which is compensated by positive (donor) charges.\(^20\) The fixed charge density at the dielectric/AlGaN interface \(n_{\text{fix}}\) can be expressed as

\[
n_{\text{fix}} = n_{2D} + \Delta \sigma_{SP, \text{diff}} - Q_g / q,
\]

where \(n_{2D}\) is 2DEG charge density, \(\Delta \sigma_{SP}\) is the net spontaneous polarization charges at AlGaN/GaN interface, \(\Delta \sigma_{SP, \text{diff}}\) is the difference of the net spontaneous polarization charges between AlGaN and GaN layers, and \(Q_g\) is the charge in the metal gate.

In the N-polar case,\(^21\) the polarization charge at the semiconductor surface is actually positive, but the net charge is negative. This leads to a charge distribution shown in Fig. 1(b). The origin of these negatively charged states in the N-polar case is not known, but we can calculate the areal density by using a similar expression as Eq. (1)

\[
n_{\text{fix}} = -n_{2D} + \sigma_{\text{polar}} - Q_g / q - F_{AlGaN} \varepsilon_{AlGaN} / q,
\]

where \(\sigma_{\text{polar}}\) is the total polarization charge at the interface in the N-polar case and \(F_{AlGaN}\) and \(\varepsilon_{AlGaN}\) are the electric field and dielectric constant in the AlGaN layer.

The explanation of interfacial fixed charge could be attributed to energy states between the conduction band minima of dielectric and AlGaN. Under both positive and
negative bias on the MIS structure, the Fermi level cannot modulate these states, and they will therefore behave like “fixed” charges. The charge density at the dielectric/AlGaN interface $n_{\text{fix}}$ plays an important role especially in scaled metal-insulator-semiconductors high-electron-mobility-transistors (MIS-HEMTs) since it acts as fixed charge which would affect electron mobility under the gate. However, in the case of conventional Schottky gate, the charges are provided by electrons in the gate metal. Since these are not randomly distributed like interface or surface states, they do not cause significant scattering.

The expression for the remote scattering rate $1/\tau_{\text{tr}}$ using a self-consistent wave function can be derived from Fermi’s golden rule as

$$\frac{1}{\tau_{\text{tr}}} = n_{\text{fix}} \frac{m^*}{2\pi\hbar^2k_F^2} \int_0^{2k_F} |V_{\text{nm}}(q)|^2 \frac{q^2dq}{\sqrt{1 - \left(\frac{q}{q_{\text{TF}}} + q\right)^2}},$$

(3)

where $m^*$ is the electron effective mass, $k_F$ and $q$ are Fermi wave factor and wave factor, respectively. $V_{\text{nm}}$ is the two-dimensional Fourier transform of the scattering potential, which can be expressed as $\frac{1}{2} \int \Delta n^* (z) n_m (z) \tilde{V} (q, z) d z$, where $\tilde{V} (q, z) = \left( \int 2\pi \delta(\omega) \right) e^{-q(z-d)}$. The distance between 2DEG and dielectric/AlGaN interface is $d$, $u_n$ and $u_m$ are the wave functions of initial and final subbands, respectively, and $\delta_q$ is the dielectric constant of GaN. The Thomas-Fermi screening effect term $q_{\text{TF}}$ is expressed as $\frac{m^*}{2\pi\hbar^2k_F^2}$. By applying the Fang-Howard approximation, the Eq. (3) can be written as

$$\frac{1}{\tau_{\text{tr}}} = n_{\text{fix}} \frac{m^*}{2\pi\hbar^2k_F^2} \left( \frac{e^2}{2\pi\epsilon_0\epsilon_R\hbar^2} \right)^2 \int_0^{2k_F} \frac{e^{-2q_d}}{q + q_{\text{TF}} G(q)} \left( \frac{b}{b + q} \right)^6 \frac{q^2dq}{\sqrt{1 - \left(\frac{q}{q_{\text{TF}}} + q\right)^2}},$$

(4)

where $b = \left( \frac{53m^*e^2n_{\text{fix}}}{9k_F\hbar^2} \right)^{1/3}$ and $G(q) = \frac{1}{8} \left( \frac{b}{b + q} \right)^3 \left( \frac{b}{b + q} \right)^2 + 3\left( \frac{b}{b + q} \right)$. The remote scattering mobility of 2DEG $\mu_{\text{remote}}$ is $\frac{e^2}{n_{\text{fix}} m^*}$, where $\tau_{\text{tr}}$ is given by the Eq. (4). We also take into account phonon scattering limited mobility at room temperature. The total mobility can be approximated as $\frac{1}{\mu_{\text{total}}} = \frac{1}{\mu_{\text{scal}}} + \frac{1}{\mu_{\text{remote}}} + \frac{1}{\mu_{\text{optical}}}$. We have used the Fang-Howard approximation to calculate the behavior of mobility as the difference in mobility between a full self-consistent wave-function, and the Fang-Howard wavefunction was not significant. From Eq. (4), the Fang-Howard wavefunction does not depend on the barrier composition, and our analysis makes the implicit assumption that there is no wavefunction extension into the barrier and hence no alloy scattering effects. This approximation is very good for high composition AlGaN or AIN barriers and when AlGaN/AIN interlayer/GaN structures are used. The details of barrier composition and thickness affect the electrostatics of the problem, and this is taken care of in our analysis from Eq. (1) by allowing $n_{\text{fix}}$ and $n_s$ to vary. Our analysis can therefore be applied to any structure if the interface charge and electron sheet charge density is known.

In Figure 2, we show the electron mobility for an oxide/2.5 nm AlGaN/GaN structure combining remote scattering and phonon scattering rates (including contributions from both optical and acoustic phonons), as a function of the 2DEG sheet charge density $n_{\text{2D}}$ assuming an impurity density of $10^{13}$ cm$^{-2}$ at the interface. At room temperature, phonon scattering dominates above the sheet carrier density of $\sim 5 \times 10^{12}$ cm$^{-2}$. The remote scattering becomes significant below this 2DEG density due to reduced screening.

To investigate the effect of scattering on 2DEG mobility in a scaled device, mobility is calculated as a function of 2DEG density for different AlGaN thickness with a fixed charge density of $1 \times 10^{13}$ cm$^{-2}$ as shown in Fig. 3. The mobility of the 30 nm AlGaN structure is not significantly impacted by remote impurity scattering due to the larger distance from the charges. However, the mobility of MIS-HEMTs with thinner AlGaN cap layers is significantly impacted, with effective mobility dropping as the sheet charge density is reduced, in which case the screening becomes less effective and scattering due to interface charge dominates. We have investigated the effect of changing fixed charge density at dielectric/AlGaN interface on the 2DEG mobility for a highly scaled device with 2.5 nm AlGaN layer, in which the scattering effect plays a huge role. Figure 4 depicts the mobility calculation result using Fang-Howard approximation with various fixed charge densities at dielectric/AlGaN interface. It is clear that the mobility is lower at
higher $n_{\text{fix}}$. As 2DEG density increases, electron mobility experiences less effect from dielectric/AlGaN interface charges as expected. In addition, the remote scattering-limited mobility becomes a dominant factor compared to phonon scattering when the interface charges increases.

The above calculations show how insulator/AlGaN interfacial charges density affect the 2DEG mobility of MIS-HEMTs. Since remote scattering is the dominant effect at low $n_{\text{2D}}$, it may not impact access regions in a device where the surface to channel distance is larger, and the charge density is high. However, the impact is more significant below the gate where the 2DEG density is reduced. In this case, 2DEG mobility under the gate indirectly impacts $f_T$ or $f_{\text{max}}$ since the mobility affects the lateral electric field distribution and velocity. In most AlGaN/GaN HEMTs, the peak $f_T$ occurs close to the pinch-off where the typical carrier concentration is between $1$ and $3 \times 10^{12} \text{cm}^{-2}$. Since this is the regime where the fixed remote charge has the greatest effect as shown in Fig. 3, we expect the scattering rate calculated here to have critical significance to understanding and improvement of the high frequency performance of highly scaled devices.

Results of this analysis can be used to select device design structures that could mitigate the effect of remote impurity scattering. While the vertical scaling necessary for high frequency transistors necessitates small gate to channel distances, tailoring the interface charge density by varying dielectric and deposition conditions could improve the mobility. Our work indicates that low interfacial fixed charge densities could greatly improve the performance of device, especially in highly vertically scaled devices.

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