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Growth and optical studies of two-dimensional electron gas of Al-rich AlGaN/GaN heterostructures

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AlGaN/GaN heterostructures were grown by metalorganic chemical vapor deposition on sapphire substrates. Time-resolved photoluminescence (PL) emission spectroscopy was employed to study the optical properties of these samples. A very strong and broad emission band was observed under high excitation intensity ($I_e = 10^4 \text{ W/cm}^2$) and its spectral peak position varies from 3.382 and 3.444 eV (at 10 K) depending on the top AlGaN layer thickness ($d$). This emission line is related to the recombination between the two-dimensional electron gas (2DEG) and photoexcited holes in AlGaN/GaN heterostructures. In a sharp contrast to the AlGAs/GaAs heterostructure system in which the PL emission line associated with the 2DEG is observable only at low temperatures ($T < 20 \text{ K}$), the 2DEG emission line in AlGaN/GaN heterostructures is observable at temperatures as high as 220 K. This is due to the strong piezoelectric polarization and deep triangular potential resulting from the large band offset in high Al content AlGaN/GaN heterostructures. For AlGaN/GaN ($x = 0.5$) heterostructures with $d = 110$ Å, five emission lines were resolved at 10 K at emission energies 70, 97, 126, 157, and 216 meV below the GaN bound exciton peak under a low excitation intensity (10 W/cm$^2$), due to the recombination between the 2DEG electrons in different subbands and photoexcited holes.

Although remarkable progress has been made in III-nitride semiconductors, Al-rich AlGaN/GaN heterostructures have been less studied and understood. Materials growth and fundamental understanding of optical and electrical properties of high Al content AlGaN/GaN heterostructures are of crucial importance for fabricating high temperature and high power electronic devices as well as optoelectronic devices. There have been a number of attempts aiming at the understanding of the transport properties of AlGaN/GaN heterostructures, but very little work, however, has been reported about the optical properties of AlGaN/GaN heterostructures and of high Al content AlGaN/GaN heterostructures in particular.

Optical properties related to two-dimensional electron gas (2DEG) in AlGaN/GaN heterostructures have been well studied. A photoluminescence (PL) peak related to 2DEG in Al$_{x}$Ga$_{1-x}$As/GaAs ($x = 0.6$) heterostructures, the $H$ band, was observable only at low temperatures ($T < 20 \text{ K}$). On the contrary, we expect to observe the PL emission line associated with the 2DEG in Al$_{x}$Ga$_{1-x}$N/GaN heterostructures, particularly in high Al content Al$_{x}$Ga$_{1-x}$N/GaN heterostructures, at higher temperatures ($T > 20 \text{ K}$), because of the strong piezoelectric field near the heterointerface as well as the strong carrier confinement resulting from the large band offset of Al$_{x}$Ga$_{1-x}$N/GaN heterostructures. Indeed, the $H$ band was observable up to 60 K in Al$_{x}$Ga$_{1-x}$N/GaN ($x = 0.22$) heterostructures.

In this letter, we present the growth and optical studies of Al$_{x}$Ga$_{1-x}$N/GaN heterostructures with $x = 0.5$. A total of five samples of Al$_{x}$Ga$_{1-x}$N/GaN heterostructures were grown by metalorganic chemical vapor deposition (MOCVD) on sapphire (0001) substrates with GaN buffer layers. These samples consist of a 1-µm-thick undoped GaN epilayer, followed by a 5-Å-thick undoped Al$_{x}$Ga$_{1-x}$N spacer layer, again followed by the top Si-doped Al$_{x}$Ga$_{1-x}$N layer with varying thickness from 55 to 140 Å. The targeted Si doping concentration for the top Al$_{x}$Ga$_{1-x}$N layer was $5 \times 10^{19}$ cm$^{-3}$. Atomic force microscopy (AFM) was employed to examine the surfaces of these samples. Variable temperature Hall measurements were used to measure the 2DEG mobility and the sheet carrier density of Al$_{x}$Ga$_{1-x}$N/GaN heterostructures. A deep UV picosecond time-resolved laser spectroscopy system was employed to study the optical properties of Al$_{x}$Ga$_{1-x}$N/GaN heterostructures.

Figure 1 presents the low temperature (10 K) PL spectra of five Al$_{x}$Ga$_{1-x}$N/GaN heterostructure samples with varying thickness ($d$) of the top Si-doped Al$_{x}$Ga$_{1-x}$N layer. Two or three peaks have been observed in each sample. The well-known donor bound exciton peak in GaN is located at 3.482 eV in each spectrum. However, another strong and broad band with spectral peak position varying from 3.382 to 3.444 eV depending on the top Al$_{x}$Ga$_{1-x}$N layer thickness is also present. We believe that this emission line is due to the recombination between the 2DEG and photoexcited holes. The general trends are that the PL emission intensity (linewidth) decreases (increases) with increasing $d$. This is due to an increased dislocation density with increasing $d$ as a result of increased lattice mismatch between Al$_{x}$Ga$_{1-x}$N and GaN. AFM studies reveal that the rms of surface morphology also increases with increasing $d$, varying from 1.5 nm for $d = 55$ Å to 2.6 nm for $d = 140$ Å, which further corroborates the PL results. However, Hall measurements revealed that the sample (KSU A-166, $d = 110$ Å) has the highest electrical quality, that is, among the different structures the sheet
conductivity was highest for this sample. Thus we have chosen the sample (KSU A-166, d = 110 Å) for more detailed PL studies, and the results are discussed below.

Figure 2 shows the PL spectra of an Al$_{0.5}$Ga$_{0.5}$N/GaN heterostructure sample with d = 110 Å measured at different temperatures from 10 to 300 K. The emission line at 3.393 eV (10 K) is attributed to the recombination between the 2DEG and photoexcited holes. Although the peak positions of both emission lines (2DEG and the I$_2$ line of GaN at 3.482 eV at 10 K) are redshifted with increasing temperature, the energy separation between the 2DEG PL peak and GaN I$_2$ peak tends to decrease with increasing temperature, which is consistent with a previous observation in low Al content (x = 0.22) Al$_x$Ga$_{1-x}$N/GaN heterostructures (T = 60 K). It is striking that the PL emission associated with the 2DEG in Al$_{0.5}$Ga$_{0.5}$N/GaN (x = 0.5) heterostructures is observable even at 220 K, while the 2DEG emission line in Al$_{0.5}$Ga$_{0.5}$As/GaAs (x = 0.6) heterostructures diminishes at temperatures greater than 20 K. This result reflects the fact that Al$_{0.5}$Ga$_{0.5}$N/GaN heterostructures have stronger piezoelectric polarizations as well as much deeper triangular potentials than Al$_{0.5}$Ga$_{0.5}$As/GaAs heterostructures, resulting from larger band offsets and lattice mismatches of Al$_{0.5}$Ga$_{0.5}$N/GaN heterostructures.

PL emission spectra of the Al$_{0.5}$Ga$_{0.5}$N/GaN heterostructure sample have been measured at 10 K under different excitation intensities (I$_{exc}$), varied over two orders of magnitude. Figure 3 shows a semilogarithmic plot of the spectral peak position (E$_p$) of the dominant 2DEG emission line as a function of excitation intensity. An approximately linear dependence of E$_p$ with log I$_{exc}$ is observed and is consistent with the result seen in low Al content Al$_x$Ga$_{1-x}$N/GaN heterostructures. Figure 4(a) shows PL emission spectrum of the Al$_{0.5}$Ga$_{0.5}$N/GaN (d = 110 Å) heterostructure under a low intensity excitation I$_{exc}$ (I$_{exc}$ = 10 W/cm$^2$) measured at 10 K. Five emission lines were observed at emission energies 70, 97, 126, 157, and 216 meV below the GaN I$_2$ peak (3.482 eV). These emission lines are due to the recombination between 2DEG electrons in different sublevels and photoexcited holes in the valence band. The solid line in Fig. 4(b) is the least squares fit of five emission energy peak positions with equation:

$$E = \left(\frac{\hbar^2}{2m}\right)^{1/3} \left[\frac{3\pi eF}{2} \left(\frac{n + \frac{3}{4}}{4}\right)^{2/3}\right] + c, \quad n = 1, 2, ..., \quad (1)$$

where $m$ is the electron effective mass, $F$ is the total electric field in the triangular potential well of Al$_{0.5}$Ga$_{0.5}$N/GaN heterostructures, $n$ is the index of the subband for electrons, and $c$ is a constant.
\( c \) is a constant which is determined by the energy gap of GaN as well as by the total band bending. The magnitude of piezoelectric field has been measured to be around 0.5 MV/cm for Al\(_{x}\)Ga\(_{1-x}\)N/GaN heterostructures. The fitted value of 90 kV/cm for this sample seems too low for the total electric field in the triangular potential in Al\(_{x}\)Ga\(_{1-x}\)N/GaN heterostructures, which we believe is due to the screening of the electrons. The screening electrons are transferred from the Si-doped AlGaN top layer to the well of Al\(_{x}\)Ga\(_{1-x}\)N/GaN heterostructures. Hall effect measurements reveal that the 2DEG sheet densities in this set of Al\(_{x}\)Ga\(_{1-x}\)N/GaN heterostructure samples are very high, around \( 1.0 \times 10^{14} \text{ cm}^{-2} \), which corroborates our charge screening explanation.

The recombination lifetimes were also measured. The inset of Fig. 5 shows the temporal responses of the PL emission measured at several different emission energies, which correspond to the recombination between the electrons and the photoexcited holes in the valence band. The total electric field of 90 kV/cm has been obtained in the triangular potential well of Al\(_{0.5}\)Ga\(_{0.5}\)N/GaN heterostructures, which shows that the effect of electron screening is very strong in Al-rich AlGaN/GaN heterostructure system.

In summary, we have investigated the growth and optical properties of Al\(_{x}\)Ga\(_{1-x}\)N/GaN heterostructures. A very strong, broad, asymmetric emission line related to 2DEG was observed in Al\(_{x}\)Ga\(_{1-x}\)N/GaN heterostructures. The 2DEG PL emission peak was observable at temperatures as high as 220 K, indicating strong piezoelectric polarization and deep triangular potential notch in Al\(_{x}\)Ga\(_{1-x}\)N/GaN (\( x = 0.5 \)) heterostructure. A total of five emission lines related with the 2DEG in Al\(_{x}\)Ga\(_{1-x}\)N/GaN (\( x = 0.5 \)) heterostructure have been observed under low laser excitation intensity, which correspond to the recombination between the electrons from different subbands (\( n = 1 \) to 5) in the conduction band and the photoexcited holes in the valence band. The total electric field of 90 kV/cm has been obtained in the triangular potential well of Al\(_{x}\)Ga\(_{1-x}\)N/GaN (\( x = 0.5 \)) heterostructures, which shows that the effect of electron screening is very strong in Al-rich AlGaN/GaN heterostructure system.

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