Raman Scattering and PL Studies on AlGaN/GaN HEMT Layers on 200 mm Si(111)


Abstract—The crystalline quality of the AlGaN/GaN high electron mobility transistor (HEMT) structure grown on a 200 mm silicon substrate has been investigated using UV-visible micro-Raman scattering and photoluminescence (PL). The visible Raman scattering probes the whole nitride stack with the Si substrate and shows the presence of a small component of residual in-plane stress in the thick GaN buffer resulting from a wafer bowing, while the UV micro-Raman indicates a tensile interfacial stress induced at the top GaN/AlGaN/AIN layers. PL shows a good crystal quality GaN channel where the yellow band intensity is very low compared to that of the near-band-edge transition. The uniformity of this sample is shown by measurements from several points across the epilayer.

Keywords—Raman, photoluminescence, AlGaN/GaN, HEMT

I. INTRODUCTION

AlGaN/GaN HEMTs are currently considered to be promising candidates in application for power devices because of the high breakdown voltage and low on-resistance [1].

The commonly used substrates for GaN epi-growth include sapphire, SiC, Si, native GaN, etc. Different from Si and GaAs whose substrates are available with a low price, GaN substrates are expensive and such a high price is caused by the difficulties associated with the formation of high-quality crystals of GaN [2]. Compared with SiC substrates which are also expensive and sapphire substrates being extensively used in LED applications, Si substrates have attracted an increasingly interest due to the much lower price and the availability of a large size substrate. However, due to the difference of lattice constants (17%) and thermal coefficients (46%) between Si and GaN, the epitaxial growth of GaN on Si (111) substrates has been proven to be difficult and metal organic chemical vapor deposition (MOCVD) is often utilized for the epitaxial process. The key issue for the process is how to properly manipulate and minimize stress during the growth to avoid cracking after cooling and also how to make the grown wafers with a low dislocation density and bowing.

In order to compensate for the disadvantages of GaN growth on Si substrates, several techniques have been adopted. AlN nucleation layers are used to avoid meltback etching effect because Ga and Si can form an alloy [3]. The graded Al$_x$Ga$_{1-x}$N intermediate layers [4-5] or AlN/GaN superlattices [6] are always used as the transitional layers between the AlN nucleation and GaN buffer layers.

Moreover, in order to make the GaN buffer layers thick enough for a high breakdown voltage application, low temperature (LT)-AIN interlayers are always inserted to manipulate the strain to avoid cracks during the growth [7-8]. Other more complex techniques such as epitaxial lateral overgrowth (ELOG) [9] and pendeoepitaxy [10] are used for a better material quality with a low dislocation density, but patterning process is needed together with two discontinuous growth processes.

Raman spectroscopy and photoluminescence (PL) techniques are used to study the vibrational and optical properties of semiconductor heterostructures. In this work, Raman spectra and PL of the AlGaN/GaN HEMT structure grown on a 200mm Si(111) substrate were examined. The uniformity was investigated with measurements from different positions in the same wafer. The residual stresses in the heterostructures and the film qualities were also studied using these nondestructive optical techniques.

II. EXPERIMENTS AND ANALYSIS

The AlGaN/GaN HEMT sample was grown by the MOCVD technique using a Veeco Turbodisc K465i tool equipped with a DRT 210 in-situ process monitor. About 140 nm AlN nucleation layer was first grown directly on a 1.05 mm thick 200 mm Si (111) substrate for avoiding the meltback etching effect. Step-graded Al$_x$Ga$_{1-x}$N intermediate layers with selective Al contents (Al$_{0.75}$Ga$_{0.25}$N~350 nm/Al$_{0.5}$Ga$_{0.5}$N~280 nm/Al$_{0.25}$Ga$_{0.75}$N~240 nm) were overgrown on the AlN layer. Then a GaN buffer layer with a thickness of ~2.5 μm was deposited while a ~10 nm LT-AIN interlayer was inserted for the purpose of strain balancing. A ~20-25 nm AlGaN barrier layer on a thin AlN spacer and a ~2 nm thin GaN cap layer were finally grown to create the two-dimensional electron gas (2DEG) heterostructure. Microscopic graphs showed that the entire 200 mm wafer is crack-free with no observable slip lines. Room temperature visible and UV Raman scattering measurements were carried out using an Ar ion laser excitation of 488 nm and a He-Cd laser operating at 325 nm, respectively. Moreover, for PL measurements, the same He-Cd laser operating at 325 nm was employed to probe the uniformity of GaN. During the optical measurements, 9 spots in different positions of the same 200 mm sample were chosen with the schematic showing the probed spots is illustrated in Fig.1. The microscopic measurements with tight focus at these probing regions avoid any spectral lineshape changes unlike mapping measurements where wafer bowing disturbs the confocality.

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Fig. 2(a) represents the semilogarithmic Raman spectrum recorded from the center position excited by 488 nm laser line. The visible Raman probes the whole nitride stack and indicates the material properties averaged over the sample layer thickness. The peaks corresponding to the Si substrate $O(\Gamma) \ (521.5 \ \text{cm}^{-1})$, GaN $E_2$-high (568.5 cm$^{-1}$), AlN:$E_2$-high (649.1 cm$^{-1}$), and GaN:$A_1$ (LO) (734 cm$^{-1}$) modes are clearly shown. The $E_2$ and $A_1$ modes of GaN are originated from the GaN buffer, while mode at 650 cm$^{-1}$ represents the $E_2$ mode from the AlN as well as Al$_x$Ga$_{1-x}$N intermediate layers. The much narrower Raman modes from GaN indicates improved crystalline quality. Typical high-resolution x-ray diffraction spectra at wafer center from these HEMT layers show a full-width at half maximum of about 540 and 670 arcsecs for the cases of (002) and (102) diffraction planes. These values indicate a high quality GaN buffer leading to much narrower $A_1$(LO) phonon line shape. The Raman spectra obtained from 9 spots across the 200 mm epilayers is demonstrated in Fig. 2(b). The $E_2$-high mode peakshift is related to the in-plane biaxial stress and appears at 568.5 cm$^{-1}$, with a no significant shift associated with measurements across the wafer. As the $E_2$(high) mode frequency of unstrained GaN at 300 K is 567.5 cm$^{-1}$, the residual in-plane stress of the GaN buffer is showing a compressive nature due to presence of a thick step-graded AlGaN intermediate layers. The in-plane stress can be calculated according to the relation between the biaxial stress and Raman peak shift [11]:

$$\Delta \omega = 4.3 \sigma_{xx} \text{cm}^{-1} \text{GPa}^{-1}$$

Therefore, the calculated stress in the GaN buffer is about -0.23 GPa. This small value of in-plane stress matches quite well with a convex wafer bowing (< 50 µm), which is also evident from the $O(\Gamma)$ phonon hardening of bulk Si. Moreover, the intensity and lineshape of $E_2$ and $A_1$ modes of GaN is similar for 9 spots, which suggest the good uniformity of GaN buffer across the epilayer. Since LO phonon lineshape is influenced by the background free carrier concentration, the characteristic of buffer is highly uniform.

In order to probe the crystalline nature of the top surface layers including AlGaN/AlN/GaN heterostructure, UV Raman measurements with an excitation wavelength of 325 nm were performed [12]. The UV Raman spectrum from the wafer center is shown in Fig. 3(a) where the peaks of GaN: $E_2$ (high) (565.5 cm$^{-1}$), two interface modes from AlGaN/AlN/GaN, and deconvoluted Al$_x$Ga$_{1-x}$N:$A_1$(LO) (768 cm$^{-1}$) are illustrated. The near-resonantly excited UV Raman probes the top 2DEG interfaces comprising of a thin 2-3 nm GaN cap and a thin AlN spacer where a sandwiched AlGaN barrier is partially strained. In this case, usage of $E_2$ peak shift in Eq (1) reveals the presence of a microscopic tensile interfacial stress and of the order of 0.47 GPa.

The interfacial stress counterbalances the wafer bowing during growth of top barrier at a lower temperature compared to higher growth temperature of AlGaN step-graded intermediate layers. Furthermore, the peak corresponding to the Al$_x$Ga$_{1-x}$N:$A_1$(LO) mode can be used to estimate the Al content $x$ by the formula when near-resonant excitation is used [13]:

$$\omega_{\text{Al}_x\text{Ga}_{1-x}\text{N}:A_1(\text{LO})} = 734 + 356.8x - 814.7x^2$$
So in the center of the wafer, the Al content is calculated to be about 14%. A slightly higher Al content is also evident at the few edges. The thickness of the AlN spacer and growth temperature of the AlGaN barrier could play important roles to enhance or reduce the Al composition pulling effect. Fig. 3(b) gives the 9 spots UV Raman spectra from the 200 mm epilayer, where we can deduce the interfacial stress at 2DEG layers and Al content to be in the range of 0.47-0.72 GPa and 14±2%, respectively. Due to a fluctuation of Al content and top AlGaN barrier thickness, the lineshape of LO phonon and interface modes shows significant changes. Since the uniformity of Al content of the barrier directly influences the 2DEG sheet carrier concentration and mobility, a further optimization of growth conditions is needed as seen from UV Raman. Nevertheless, such layering has resulted in room-temperature electron mobility of about 1800 cm²/Vs as seen from Hall effect measurements in such HEMT wafers.

The room-temperature PL spectra recorded from 9 spots were also measured as shown in Fig. 4. From the plots, the dominant peaks under 325 nm excitation are represented by the near-band-edge (NBE) transitions of GaN located at the same peak energy of 3.41 eV. No significant peak shift is detected, thus results showing the uniformity of GaN channel regions. Compared to the intensity of NBE transition, the yellow luminescence band (YL) is not significant. The YL is related to deep level emissions associated with vacancy-impurity complexes. The NBE to YL intensity ratio is similar for all 9 spots, which indicate the uniformity and good crystalline quality GaN.

![Fig. 3 UV Raman Spectra of the sample. (a) UV Raman spectrum from the wafer center; (b) Raman spectra recorded from 9 points across the wafer as shown in Fig. 1. The spectra are shifted horizontally for clarification (The sequence of curves of the center to Tedge is from bottom to top)](image)

![Fig. 4 Semilogarithmic PL spectra obtained from 9 spots across the 200 mm epilayer)](image)

### III. Conclusion

A detailed study on Raman spectroscopy of AlGaN/GaN HEMT layers grown on 200 mm Si (111) substrate is presented. Using the visible Raman spectra at 488 nm excitation, a compressive residual stress of the order of 0.23 GPa is probed, which is linked to a convex wafer bowing. However, due to the presence of a thin AlN spacer beneath AlGaN barrier, the UV Raman probes the microscopic interfacial stress which influences the 2DEG properties. From the deconvoluted AlₙGa₁₋ₙN:Al⁺ (LO) modes obtained from 9 spots across the wafer by UV Raman, the Al content in the top AlGaN barrier is determined. The PL spectra indicate that the epilayer has a good crystal quality and uniform GaN channel. The layers are suitable for high voltage electronic devices.

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