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Surface Passivation of AlGaN/GaN Heterostructures Using An Ultrathin Al₂O₃ Layer

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We demonstrate a novel surface passivation process for AlGaN/GaN heterostructures utilizing an ultrathin Al₂O₃ layer (~1 nm). The Al deposition and the thermal annealing processes in UHV were found to form the ultrathin Al₂O₃ layer on the surface of the AlGaN/GaN heterostructure, which was confirmed by *in-situ* x-ray photoelectron spectroscopy (XPS) analysis. The reverse leakage current for the Schottky gate contact on the Al₂O₃-passivated heterostructure surface was reduced by three orders of magnitude than that for the conventional Schottky gate structure. C-V results showed good gate controllability of two-dimensional electron gas (2DEG) by the novel gate structure.

1. Introduction

The AlGaN/GaN heterostructure field effect transistors (HFETs) have been key electronic devices for high-power applications at microwave/millimeter-wave frequencies. Although there have been a lot of reports on excellent frequency and power performances of AlGaN/GaN HFETs, they have suffered from surface/interface-related problems. For example, they have a large gate leakage current [1, 2], aging of Schottky contacts to AlGaN [3] and frequency dispersion in drain current [4], etc. In order to overcome these problems, it is essentially indispensable to understand the AlGaN/GaN heterostructure surfaces and to realize a suitable surface passivation process.

In this paper, we demonstrate a novel surface passivation process for AlGaN/GaN heterostructures utilizing an ultrathin Al₂O₃ layer. The formation process of an ultrathin Al₂O₃ layer was characterized and optimized by x-ray photoelectron spectroscopy (XPS) method. The passivation effect of an ultrathin Al₂O₃ layer was examined in terms of current-voltage (I-V) and capacitance-voltage (C-V) characteristics for the metal/ultrathin-Al₂O₃/AlGaN gate structure.

2. AlGaN/GaN heterostructure sample

The AlGaN/GaN heterostructure wafers grown on (0001) sapphire substrates by metalorganic vapor phase epitaxy (MOVPE), as shown in **Fig. 1**, were used in this study. The Hall mobility and sheet carrier concentration of the two-dimensional electron gas (2DEG) formed at the AlGaN/GaN heterointerface were 1300 cm²/Vs and 1.5 x 10¹³ cm⁻² at room temperature (RT), and 5700 cm²/Vs and 1.2 x 10¹³ cm⁻² at 77 K, respectively.

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Al _{0.25} Ga _{0.75} N (3 nm)
n ⁺ -Al _{0.25} Ga _{0.75} N (25 nm)
Al _{0.25} Ga _{0.75} N (3 nm)
2DEG
GaN (2 μm)
GaN LT buffer (20 nm)
Sapphire substrate

Fig. 1. The AlGaIn/GaN heterostructure sample

3. Results and Discussion

3.1 XPS analysis on passivated AlGaIn/GaN heterostructure surfaces

Detailed XPS analysis showed that the air-exposed AlGaIn/GaN heterostructure surface possessed highly non-stoichiometric phase with large amounts of natural oxide [5, 6]. The wet chemical treatment in the NH₄OH solution at 50°C was found to be very effective in reducing the natural oxide layer on the surface of the as-grown AlGaIn/GaN heterostructure wafer. However, there remained a small amount of natural oxide including Al₂O₃ and Ga₂O₃ components even on the NH₄OH-treated surface.

To control such a surface, we attempted to form an ultrathin Al₂O₃ passivation layer by the following process. First, ultrathin (1 nm) Al layer was deposited on the NH₄OH-treated AlGaIn surface at RT using a K-cell with a rate of 0.01 nm/s in an MBE chamber (3×10^{-10} Torr). Then, the sample was annealed at 800°C for 10 min in UHV annealing system. The basic idea of this process is to convert the natural oxide on the AlGaIn surface to the Al oxide (Al₂O₃) by use of the reaction with an active metallic Al. The novel passivation process was optimized by *in-situ* XPS analysis.

Figure 2(a) shows *in-situ* XPS Al2p spectra taken from the Al-deposited surface with escape angle of 10° and 60°. The Al-O bonding peaks were detected in addition to the metallic Al and AlGaIn peaks, in spite of the fact that the Al deposition was done in UHV. From the angle-resolved XPS analysis of the Al2p peak, an Al-oxide was found to grow at the Al/AlGaIn interface, indicating the reaction between metallic Al and residual natural oxide during the deposition process. After the UHV anneal at 800°C for 10 min, the metallic Al peak disappeared in the Al2p spectra, as shown in Fig. 2(b). The Al2p spectra could be deconvoluted into the two peaks assigned to the bulk AlGaIn peak and the topmost Al-oxide peak. The Al-O bonding peak position is very close to that of the Al₂O₃ phase. The integrated intensity ratio of the O1s/Al2p(Al-O) was 5.7, also close to the value of reference sapphire (Al₂O₃) substrate. In addition, the peak intensity of Ga₂O₃ component in the Ga3d spectra was found to decrease after the UHV annealing process. Thus, this annealing process enhanced the reaction between metallic Al and residual natural oxide, resulting in the formation of the ultrathin Al₂O₃ layer. The thickness of the ultrathin Al₂O₃ layer was estimated to be 1.2 nm.

Figure 3(a) shows the XPS O1s spectrum obtained from the Al₂O₃/AlGaIn sample. The energy loss signal exhibited a rather broad peak at the higher binding energy side away from the O1s core-level energy position. From the onset of the O1s energy loss signal seen in Fig. 3(b), the energy gap (E_g) of the ultrathin Al₂O₃ layer was estimated to be 6.1 eV, suitable for a surface passivation of AlGaIn ($E_g \sim 4.0$ eV). Almost the same value for the Al₂O₃ film on the

Si (100) substrate was reported by Itokawa *et al.* [7].

Fig. 2. XPS Al_{2p} spectra of the NH_4OH -treated surface with escape angle of 10° and 60° after (a) the Al deposition at RT and (b) subsequent UHV annealing at 800°C for 10 min.

Fig. 3. (a) The XPS $\text{O}1s$ spectrum obtained from the $\text{Al}_2\text{O}_3/\text{AlGaN}$ sample and (b) the energy loss spectrum with respect to the $\text{O}1s$ core-level position

3.2 Electrical properties of Pt Schottky contacts to the ultrathin- Al_2O_3 passivated surfaces.

The passivation effect of the ultrathin Al_2O_3 layer was examined in terms of I-V and C-V characteristics for the novel Pt/ Al_2O_3 Schottky gate structure. The ring-shaped Ti/Al/Ti/Au ($\approx 20/80/20/50$ nm) ohmic electrodes were formed on the heterostructure surface, which surrounded the Pt gate electrode. The annealing of the ohmic contacts was performed at 600°C for 2 min in N_2 ambient.

Figure 4 compares the I-V characteristics for the novel Pt/ Al_2O_3 and the conventional Pt Schottky gate structures. The novel gate structure showed relatively small ideality factor of 1.17, similar to the conventional Schottky gate contact. This indicated that the current transport basically through the Schottky barrier was not significantly modified by the insertion of the ultrathin Al_2O_3 layer because the Al_2O_3 layer is very thin (~ 1 nm). For the conventional Schottky gate sample, the I-V characteristics exhibited the very leaky (ohmic-like) behavior in the bias region from -0.1 V to 0.1 V. In comparison, the rectifying characteristic was significantly improved for the novel Pt/ Al_2O_3 structure, as shown in the dotted curve in Fig. 4. Furthermore, the reverse gate leakage current at $V_g = -5$ V was reduced by three orders of magnitude than the conventional Schottky gate structures.

From the C-V measurement, we evaluated the controllability of the depletion layer for

the Pt/Al₂O₃ gate structure. The obtained capacitance value at zero bias was in agreement with the calculated one from the thickness of AlGa_{0.3}N layer (31 nm). No noticeable hysteresis and frequency dispersion were observed in C-V characteristics at 10 kHz-1MHz, and clear pinch-off behavior was obtained. These results indicated that the good gate control of the depletion layer at AlGa_{0.3}N/GaN heterointerface was achieved by the present Pt/Al₂O₃ gate structure.

Fig.4 The I-V characteristics for (a) a conventional Schottky and (b) a novel Pt/ Al₂O₃ gate structures

4. Conclusion

A novel surface passivation process for AlGa_{0.3}N/GaN heterostructures utilizing an ultrathin Al₂O₃ layer was demonstrated. The combination of the Al deposition and the annealing processes in UHV achieved the formation of the ultrathin Al₂O₃ layer on the surface of the AlGa_{0.3}N/GaN heterostructure. The formation process of the Al₂O₃ passivation layer was optimized by in-situ XPS. The reverse gate leakage in the novel Pt/Al₂O₃ gate structure was reduced by three orders of magnitude than the conventional Pt Schottky structure. In addition, the Pt/Al₂O₃ gate structure exhibited good gate controllability of 2DEG. Thus the present passivation process is promising for realizing reproducibility of device fabrication process and reliability of device operation.

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