Investigation of Oxygen Incorporation in AlGaN/GaN Heterostructures

Ho Won Jang, Jeong Min Baik, Jong-Lam Lee, Hyun-Joon Shin, and Jung-Hee Lee

Abstract— **Direct evidence on the incorporation of high concentration of oxygen into undoped AlGaN layers for the AlGaN/GaN heterostuctures is provided by scanning photoemission microscopy using synchrotron radiation. *In-situ* annealing at 1000 °C resulted in a significant increase in the oxygen concentration at the AlGaN surface due to the predominant formation of Al-O bonds. The oxygen incorporation into the AlGaN layers resulting from the high reactivity of Al to oxygen can enhance the tunneling-assisted transport of electrons at the metal/AlGaN interface, leading to the reduction of the Schottky barrier height and the increase of the sheet carrier concentration near the AlGaN/GaN interface.**

Index Terms— **AlGaN/GaN heterostructures, oxygen, unintentional doping, SPEM**

I. INTRODUCTION

AlGaN/GaN heterostructures are promising materials for high power, high temperature electronic devices such as heterostructure field effect transistors and heterojunction bipolar transistors [1,2]. One of the most important characteristics of AlGaN/GaN heterostructures is ability to achieve to achieve two-dimensional electron gas (2DEG) higher than 10^{13} cm^{-2} at the interface of AlGaN with GaN even in no intentional doping [3]. Recent works showed that the creation of such high density of 2DEG in AlGaN/GaN heterostructures originates predominantly from the existence of donors-like defects in the AlGaN layers, such as nitrogen vacancies, oxygen impurities, and surface donors [4-6].

For GaAs/AlGaAs heterostructure devices, it is well known that the unintentional incorporation of oxygen into AlGaAs layers is detrimental to device performance because of the generation of midgap electron traps such as DX centers [7,8]. However, in the AlGaN/GaN heterostructures, few works have reported on the effect of oxygen incorporation on device performance. One possible reason is due to lack of study on the mechanism for the unintentional incorporation of oxygen into the AlGaN layers.

In this letter, we report an investigation on oxygen incorporation into AlGaN layers for AlGaN/GaN heterostructures using scanning photoemission microscopy (SPEM). *In-situ* vacuum annealing and subsequent SPEM imaging accompanied with space-resolved photoemission spectroscopy (SRPES) provide direct evidence on the predominant oxygen incorporation into the AlGaN layers. Finally, the influence of the high oxygen content in the AlGaN layers on the electrical properties of the heterostuctures is discussed.

II. EXPERIMENT

AlGaN/GaN heterostructure films used in this work were grown on (0001) sapphire substrate using metalor-

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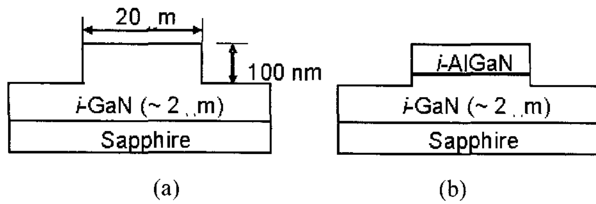

Fig. 1. Schematic illumination of the (a) GaN and (b) AlGaN/GaN samples with 20-μm-width line patterns for SPEM measurements.

ganic chemical-vapor deposition. Two types of sample were prepared. The first is an undoped GaN sample with a thickness of 2.0 μm as a reference. The second is an AlGaN/GaN heterostructure with a 450-Å-thick undoped $Al_{0.34}Ga_{0.76}N$ layer grown on the undoped GaN sample. The carrier density and electron mobility of the samples were measured to be 8×10^{16} cm^{-3}, 150 cm^2/Vs for the GaN sample, and 2.3×10^{13} cm^{-3}, 1070 cm^2/Vs for the AlGaN/GaN sample, respectively. In order to observe oxygen incorporation into GaN and AlGaN layers clearly using SPEM, line patterns with a 20 μm width were defined by Cl_2/BCl_3 inductively coupled plasma (ICP) etching, as shown in Fig. 1. After the dry etching, the samples were dipped into a boiling $HCl:HNO_3$ (3:1) solution for 10 min to remove surface contamination [9].

SPEM measurements were carried out at the 8A1 undulator beamline at the Pohang Accelerator Laboratory (PAL) [10]. The lateral-space resolution is determined by the size of the zone-plate focused x-ray beam, which is 0.4-0.5 μm with a photon flux of 5.3×10^7-10^8 photons/s. A hemispherical electron energy analyzer collects and analyzes the photoelectrons. The analyzer has 16 energy-detecting channels/windows, and the energy separation/resolution per window is 0.8 eV. Taking multi-images at different photoelectron energies, we simultaneously obtained SRPES spectra at selected points.

III. Results and Discussion

Figure 2 shows O 1*s* SPEM images and SREPS spectra for the GaN and AlGaN/GaN samples. In the SPEM image of the GaN sample, the unetched GaN area appeared brighter than the etched region, indicating that the concentration of surface oxygen is higher in the

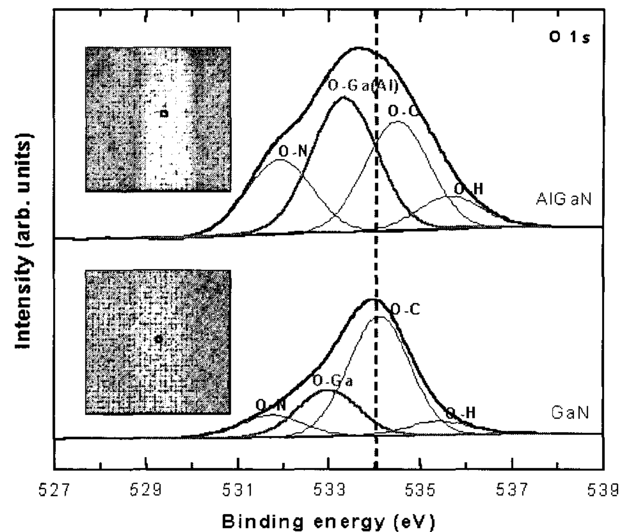

Fig. 2. O 1s SPEM images and SREPS spectra for the GaN and AlGaN/GaN samples. The image size is 50 × 50 μm2. The SRPES spectra were obtained at the binding energy of 534 eV on the unetched regions indicated by the circles.

unetchecd GaN sample. This is due to the fact that the ICP dry etching effectively removes oxycarbon contaminates (C-O). For the AlGaN/GaN sample, the contrast of O 1*s* signal between the unetched and etched areas became more pronounced. This means that the oxygen concentration in the surface of AlGaN is much higher than that in the surface of GaN, in good agreement with the previous result [6]. In order to identify the chemical bonding states of oxygen at the surface region, O 1*s* core level spectra were obtained at the unetched GaN and AlGaN surfaces. For the GaN sample, the O 1*s* peak was deconvoluted into four bonds corresponding to O-N, O-Ga, O-C, and O-H bonds, respectively. The binding energy differences are in good agreement with previously reported values [11-13]. According to the previous studies on surface oxides on GaN, oxynitride phase (Ga-O-N), the intermediate phase between oxide (G-O) and nitride (Ga-N) can exist on the GaN surface [14]. Thus the peak located at 531.7eV with the binding energy difference of 1.25 eV from the O-Ga bond was determined to be the O-N bond. In the AlGaN surface, the O 1*s* peak was also deconvoluted into the four bonds. Compared to the O 1*s* peak in the GaN sample, the increase in the O-Ga(Al), O-N, and O-H bonds is more dominant rather than that in the O-C bond. Although the peak separation of the O-Ga(Al) into O-Ga and O-Al bonds is difficult due to the almost same binding ener-

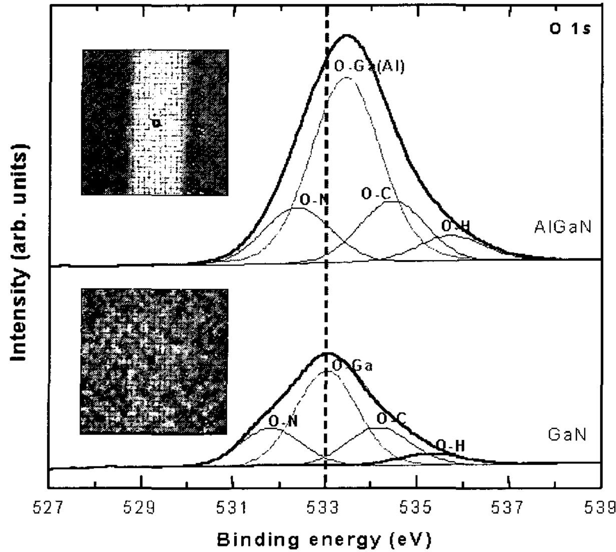

Fig. 3. O 1s SPEM images and SREPS spectra for the GaN and AlGaN/GaN samples after annealing at 1000 oC for 2 min. The image size is 50 × 50 µm2. The SRPES spectra were obtained at the binding energy of 533 eV on the unetched regions indicated by the circles.

Table I. The relative atomic concentration (%) at the GaN and AlGaN surfaces before and after the high temperature annealing.

		Ga		Al		N	O	C
		Ga-N	Ga-O	Al-N	Al-O			
GaN	Before	48.0	5.4	-	-	11.0	9.0	26.6
	After	50.5	8.5	-	-	18.4	18.6	4.0
AlGaN	Before	25.2	4.2	19.8	3.4	12.9	10.0	25.5
	After	25.1	3.2	10.4	16.4	13.9	27.6	3.4

gies, it could be deduced that the higher oxygen concentration at the AlGaN surface is attributed to the presence of Al due to high reactivity of Al to oxygen. The binding energy difference between two samples originates from the difference of bandgap energy between GaN and $Al_{0.34}Ga_{0.66}N$ (0.72 eV).

In order to clarify the high oxygen content at the AlGaN surface, the samples was cleaned through *in-situ* annealing at 1000 °C for 2 min. The annealing temperature was selected to be close to the growth temperature of both AlGaN and GaN layers (~1050 °C). During the annealing, the base pressure was controlled to be lower than 1 × 10^{-6} Torr.

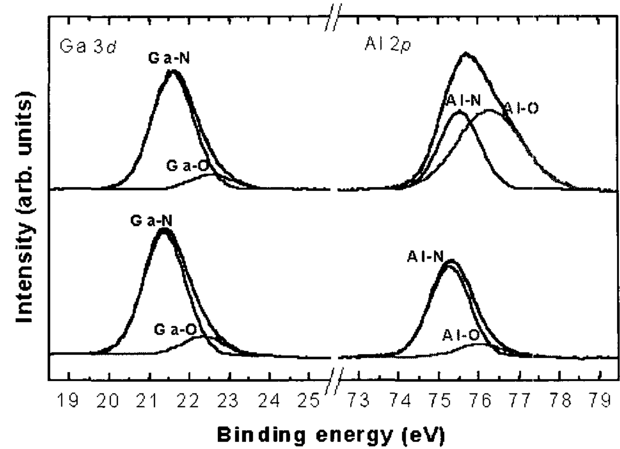

Fig. 4. SRPES spectra of (a) Ga 3d and (b) Al 2p core levels for the AlGaN surface before and after the high temperature annealing.

Figure 3 shows O 1*s* SPEM images and SREPS spectra for the GaN and AlGaN/GaN samples after the high temperature annealing. It is noteworthy that the image contrast in the AlGaN/GaN sample became more pronounced, while there was no contrast in the GaN sample. This indicates that the high temperature annealing induced a significant increase in oxygen content at the AlGaN surface region, as shown in Table I. The O 1*s* spectra show that the increase of the oxygen concentration was mainly due to the increase in the peak intensity of the O-Ga and/or O-Al bonds.

Figure 4 shows SRPES spectra of Ga 3*d* and Al 2*p* core level for the AlGaN surface before and after the high temperature annealing. In the peak fitting of the spectra, two main components of Ga-N (Al-N) and Ga-O (Al-O) bonds were considered, assuming that the Ga-O-N and Al-O-N bonds could be superimposed into the deconvoluted Ga-O and Al-O bonds, respectively. The change in the peak intensity ratio of $I_{Ga\text{-}O}/I_{Ga\text{-}N}$ was negligible after the annealing. However, the ratio of $I_{Al\text{-}O}/I_{Al\text{-}N}$ increased significantly, indicating the predominant formation of the Al-O bond during the *in-situ* annealing. This result provides direct evidence on the high reactivity of Al to oxygen at the AlGaN surface. Therefore, it could be concluded that the unintentional incorporation of oxygen into AlGaN layers during epitaxial growth originates from the high reactivity of Al to oxygen.

In order to confirm the unintentional incorporation of oxygen into AlGaN layers, secondary ion mass spectroscopy (SIMS) was carried out, as shown in Fig. 5.

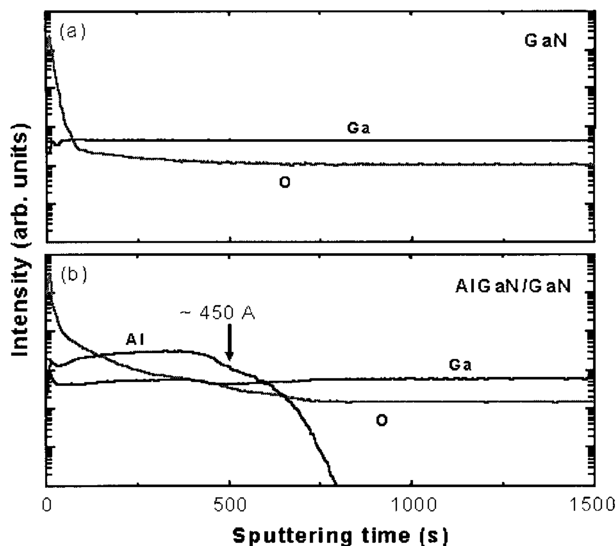

Fig. 5. SIMS depth profiles of the as-grown (a) GaN and (b) AlGaN/GaN samples.

In the undoped GaN sample, the high concentration of oxygen near the surface region was observed, corresponding to the surface oxide layer. In the undoped AlGaN/GaN sample, it was founded that the oxygen depth profile tapered beyond the AlGaN/GaN interface. The average concentration of oxygen in the AlGaN layer is higher by one order of magnitude than that in the GaN layer. This result shows that a large amount of oxygen is incorporated into the AlGaN layers and exists predominantly near the surface region.

Finally, the effect of the oxygen incorporation into the AlGaN layer on electrical properties of metal contacts to the AlGaN/GaN sample was investigated, as shown in Fig 6. For Pt Schottky diodes, the rectifying characteristic of the Schottky contact was pronounced in the GaN sample. The reverse leakage current at -10 V in the AlGaN/GaN sample was higher by five orders of magnitude than that in the GaN one. The values of Schottky barrier height and ideality factor determined using the thermionic emission model were respectively 1.04 eV and 1.24 for the GaN sample, and 0.83 eV and 2.34 for the AlGaN/GaN sample. The higher Schottky barrier height and the lower ideality factor in the AlGaN/GaN sample imply that the carrier transport mechanism was modified from the thermionic emission. Current-voltage (*I-V*) characteristics of as-deposited Ti/Al ohmic contacts were shown in Fig. 6(b). The *I-V* curve for the GaN sample was completely rectifying, while the AlGaN/GaN sample showed ohmic behavior.

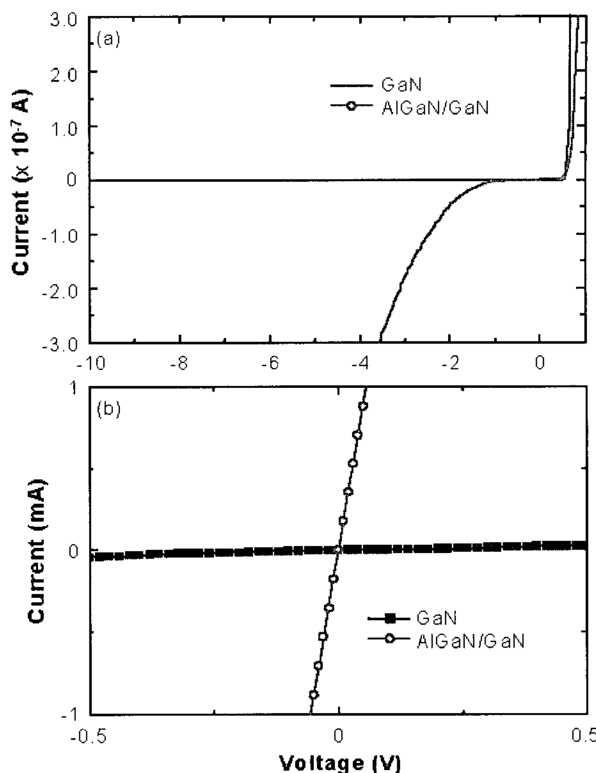

Fig. 6. I-V characteristics of (a) Pt Schottky diodes and (b) nonalloyed Ti/Al ohmic contacts on the GaN and AlGaN/GaN samples.

Specific contact resistivity was determined to be $1.2 \times 10^{-3}\ \Omega\ cm^2$. This result indicates that the tunneling-assisted current across the metal/AlGaN interface should be very high.

The dominant incorporation of oxygen into the AlGaN layer was observed using SPEM measurements. The Gibbs free energy change in the transformation of Al into Al oxide (Al_2O_3) is -1262 kJ/mol, but -665 kJ/mol in the transformation of Ga into Ga oxide (Ga_2O_3) [15]. Thus, when oxygen atoms are collided onto the film surface during epitaxial growth [16], the probability of chemisorption into the surface layer can increase with the Al content. As a result, the number of oxygen atoms occupying N atomic sites is higher in the AlGaN layer than that in the GaN layer. Because oxygen is a shallow donor with ionization energy of 32 ~ 37 meV [17], the AlGaN layer containing oxygen changes into an n-type semiconductor. As shown in Fig. 4, since the oxygen atoms exist predominantly near the surface region, near-surface region becomes a degenerated AlGaN layer. As a result, the band bending in the AlGaN layer doped with oxygen donors became steep below the surface. This

enhanced tunneling-assisted transport of electrons at the interface of the AlGaN with metal contacts, resulting in the decrease in both the Pt SBH and the contact resistivity of the nonalloyed Ti/Al contact, as shown in Fig. 6. In addition, the band bending in the highly doped AlGaN layer provides very efficient transfer of electrons to the GaN well, increasing the electron density of the two-dimensional electron gases (2DEG) at the AlGaN/GaN heterointerface [18].

IV. Conclusoin

We investigated the mechanism for the oxygen incorporation into the AlGaN layers for AlGaN/GaN heterostuctures using scanning photoemission microscopy (SPEM). *In-situ* vacuum annealing at 1000 °C and subsequent SPEM imaging provided direct evidence on the oxygen incorporation into the AlGaN layers originating form the high reactivity of Al to oxygen. Predominant incorporation of oxygen donor impurities near the surface region of AlGaN led to the enhanced tunnelling-assisted transport of electrons across the metal/AlGaN interface and the increased 2DEG density at the heterointerface.

Acknowledgement

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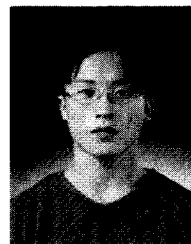
References

[1] O. Ambacher *et al.*, J. Phys.: Condens. Matter 14, 3399 (2002).
[2] C.R.Abernathy *et al.*, J. Semicond. Tech. Sci. 3, 13 (2003).
[3] P. M. Asbeck, E. T. Yu, S. S. Lau, G. J. Sullivan, J. Van Hove, and J. Redwing, Electron. Lett. 33, 1230 (1997).
[4] I. P. Smorchkova, C. R. Elsass, J. P. Ibbetson, R. Vetury, B. Heying, P. Fini, E. Haus, S. P. DenBaars, J. S. Speck, and U. K. Mishra, J. Appl. Phys. 86, 4520 (1999).
[5] J. P. Ibbetson, P. T. Fini, K. D. Ness, S. P. Denbaas. J. S. Speck, and U. K. Mishra, Appl. Phys. Lett. 77, 250 (2000).
[6] H. W. Jang, C. M. Jeon, K. H. Kim, J. K. Kim, S.-B. Bae, J. -H. Lee, J. W. Choi, and J.-L. Lee, Appl. Phys. Lett. 81, 1249 (2002).
[7] K. A. Prior, G. J. Davies, and R. Heckingbottom, J. Cryst. Growth 66, 55 (1984).
[8] C. Amano, K. Ando, and M. Yamaguchi, J. Appl. Phys. 63, 2853 (1988).
[9] J. K. Kim, J. L. Lee, J. W. Lee, H. E. Shin, Y. J. Park, and T. Kim, Appl. Phys. Lett. 73, 2953 (1998).
[10] T. Mattila and R. M. Nieminen, Phys. Rev. B 55, 9571 (1997).
[11] I. Shalish, Y. Shapira, L. Burstein, and J. Salzman, J. Appl. Phys. 89, 390 (2001).
[12] J. F. Mouler, W. F. Strickle, P. E. Sobol, and K. D. Bomben, *Handbook of X-Ray Photoelectron Spectroscopy*(Perkin-Elmer, Eden Prairie, MN, 1992).
[13] H. W. Jang, J. K. Kim, J.-L. Lee, J. Schroeder, and T. Sands, Appl. Phys. Lett. 82, 580 (2003).
[14] S. D. Walter, J. M. DeLucca, S. E. Mohney, R. S. Kern, and C. P. Cuo, Thin Solid Films 371, 153 (2000).
[15] B. Ihsan, *Thermochemical Data of Pure Substances* (VCH Publishers, New York, NY, 1987).
[16] C. R. Elsass, T. Mates, B. Heying, C. Poblenz, P. Fini, P. M. Petroff, S. P. DenBaars, and J. S. Speck, Appl. Phys. Lett. 77, 3167 (2000).
[17] W. Gotz, N. M. Johnson, C. Chen, H. Liu, C. Kuo, and W. Imler, Appl. Phys. Lett. 68, 3144 (1996).
[18] O. Ambacher *et al.* J. Appl. Phys. 87, 334 (2000).



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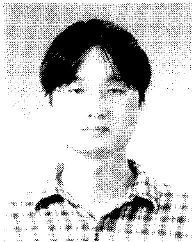

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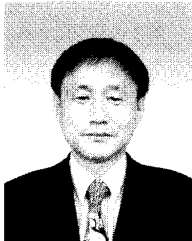

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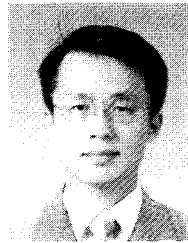

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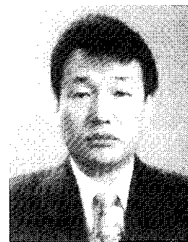

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