Schottky Contacts to Polar and Nonpolar n-type GaN

Hogyoung Kim*

College of Humanities and Sciences, Hanbat National University, Daejeon 305-719, Korea

Soo-Hyon Phark

Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Keun-Man Song

Korea Advanced Nano Fab Center, Suwon 443-270, Korea

Dong-Wook Kim

Department of Physics, Department of Chemistry and Nano Science, Ewha Womans University, Seoul 120-720, Korea

(Received 15 June 2011)

Using the current-voltage measurements, we observed the barrier heights of c-plane GaN in Pt and Au Schottky contacts to be higher than those of a-plane GaN. However, the barrier height of c-plane GaN was lower than that of a-plane GaN in the Ti Schottky contacts. The N/Ga ratio calculated by integrating the X-ray photoelectron spectroscopy (XPS) spectra of Ga 3d and N 1s core levels showed that c-plane GaN induced more Ga vacancies near the interface than a-plane GaN in the Ti Schottky contacts, reducing the effective barrier height through an enhancement of the tunneling probability.

PACS numbers: 85.30.De, 85.60.-q, 81.05.Ea

Keywords: Schottky contacts, Nonpolar GaN, Ga vacancies

DOI: 10.3938/jkps.60.104

I. INTRODUCTION

GaN and related nitride semiconductors have gained considerable attraction due to their applications in light-emitting diodes (LEDs), blue/ultraviolet lasers, and high-power/high-temperature electronic devices [1]. However, the performance of these devices fabricated using conventional c-plane GaN layers has been limited by spontaneous and piezoelectric polarizations due to the quantum-confined Stark effect [2,3]. Polarizationinduced electric fields cause a spatial separation of the electron and the hole wave functions in the quantum well (QW), reducing the luminescence efficiency and shifting the light emission to longer wavelengths than in polarization-free structures [4]. The problem of these polarization-related effects in nitride-based devices can be solved using nonpolar GaN films such as a- or mplane [5,6]. However, nonpolar GaN films typically have highly extended defect densities, such as threading dislocations and basal plane stacking faults [7].

For the fabrication of nonpolar GaN-based devices, it

is essential to understand the electrical properties of the metal contacts to GaN. Adivarahan et al. reported that Pd Schottky contacts to a-plane GaN prepared by epitaxial lateral overgrowth (ELO) have a barrier height of 0.4 eV and an ideality factor of 1.1 [8]. The lower barrier height of a-plane GaN compared to that of c-plane GaN was found in Pd and Pt Schottky contacts to GaN [9,10]. The sheet resistance of a-plane GaN along the caxis was observed to be two times higher than that along the m-axis, which shows significant electric anisotropy in the two orientations [11]. Nanoscale electrical characterization of nonpolar GaN using scanning capacitance microscopy and conductive atomic force microscopy (C-AFM) has also been attempted to find the correlation between surface defects and electrical behaviors [12]. More research is required to fully understand the electrical behaviors of metal contacts to nonpolar GaN. In this work, we investigated the electrical properties of Schottky contacts to c- and a-plane n-type GaN using Pt, Au, and Ti electrodes.

^{*}E-mail: hogyoungkim@gmail.com; Fax: +82-42-821-1599

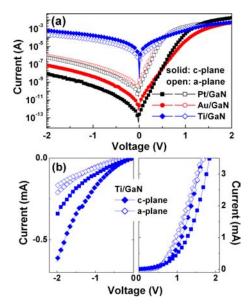


Fig. 1. (Color online) (a) Semilogarithmic current-voltage (I-V) characteristics for the Pt, Au and Ti Schottky contacts to c- and a-plane n-type GaN and (b) linear I-V characteristics of Ti/GaN Schottky diodes.

II. EXPERIMENTS

Polar c-plane (0001) and nonpolar a-plane (11 $\bar{2}0$) ntype GaN thin films were grown by using metalorganic chemical vapor deposition (MOCVD) on c-plane and rplane $(1\bar{1}02)$ sapphire substrates, respectively. The carrier concentration and the mobility assessed by using Hall-effect measurements were $1.40 \times 10^{18} \text{ cm}^{-3}$ and 302 ${\rm cm^2/V \cdot s}$ for c-plane GaN and $1.43 \times 10^{18}~{\rm cm^{-3}}$ and 53 cm²/V⋅s for a-plane GaN. Planar Schottky diodes were fabricated using standard photolithography. The samples were cleaned in acetone and methanol, and the surface oxide was removed in a HCl:H₂O (1:1) solution immediately prior to loading into an electron-beam evaporator. A Ti/Al (30 nm/110 nm) bilayer was deposited to serve as the ohmic contact, followed by rapid thermal annealing at 400 °C for 1 min in an N₂ ambient. Then, Pt, Au, and Ti metals were deposited for the Schottky contacts. Current-voltage (I-V) measurements were performed using a semiconductor parameter analyzer (HP 4156B). X-ray photoelectron spectroscopy (XPS) measurements were carried out using a monochromatic Mg $K\alpha$ X-ray source to explore the metal-GaN contact formation mechanisms.

III. RESULTS AND DISCUSSION

Figure 1(a) shows the I-V characteristics of Pt, Au and Ti Schottky contacts formed on c- and a-plane n-type GaN. The electrical parameters were obtained with the I-V method, which utilizes a large-area contact and

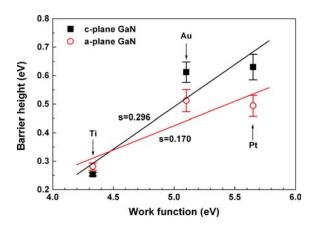


Fig. 2. (Color online) Effective barrier heights for the Pt, Au, and Ti contacts to c- and a-plane n-type GaN as functions of their corresponding metal work function. Sold lines represent the linear fits to the experimental data and were used to extract the density of interface states.

reverse-biased I-V characteristics given by [13]

$$I = I_0 \exp(qV/nk_BT)[1 - \exp(-qV/k_BT)],$$
 (1)

$$I_0 = AA^{**}T^2 \exp(-q\phi_B/k_BT),$$
 (2)

where A is the device area, A^{**} is the effective Richardson constant, assumed to be 26.4 A/cm²K² for n-type GaN [14], n is the ideality factor, ϕ_B is the effective barrier height, and V is the applied voltage. The analyses for the Pt Schottky contacts revealed that $\phi_B =$ $0.63~(\pm 0.05)~{\rm eV}~{\rm and}~n=1.29~(\pm 0.08)~{\rm for~the}~c\text{-plane}$ GaN sample and $\phi_B = 0.49 \ (\pm 0.04) \ \text{eV}$ and n = 1.24 (± 0.02) for the a-plane GaN sample. Likewise, the analyses of the Au Schottky contacts showed that $\phi_B = 0.61$ (± 0.04) eV and n = 1.30 (± 0.06) for the c-plane GaN sample and $\phi_B = 0.51 \; (\pm 0.04) \; \text{eV} \; \text{and} \; n = 1.23 \; (\pm 0.02)$ for the a-plane GaN sample. Compared to the contacts on the c-plane GaN, those on the a-plane GaN had lower barrier heights. That phenomenon was attributed to the absence of polarization-induced surface charges for the a-plane GaN [9]. ϕ_B and n of the Ti Schottky contacts were found to be 0.25 (± 0.02) eV and 1.19 (± 0.02) for c-plane GaN and 0.29 (± 0.01) eV and 1.24 (± 0.02) for a-plane GaN. Although the difference is small, c-plane GaN has a lower barrier height than a-plane GaN for the Ti Schottky contacts, different from the Pt and the Au Schottky contacts. The reason will be discussed later.

Figure 2 shows the effective barrier heights for the Pt, Au and Ti Schottky contacts as functions of their corresponding metal work function. As can be seen in this plot, the dependence of the barrier heights on the metal work function is smaller for the a-plane GaN than for the c-plane GaN. If the density of interface states is assumed to be uniform and is not disturbed by the metal deposition, the following formula developed by Cowley

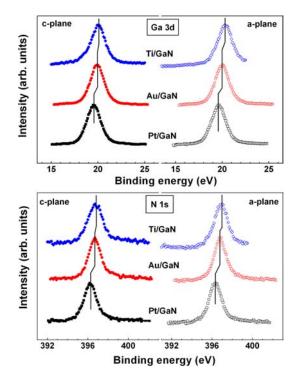


Fig. 3. (Color online) XPS spectra of Ga 3d and N 1score levels for the Pt, Au, and Ti contacts to c- and a-plane n-type GaN.

and Sze can be used [15]:

$$\phi_{Bn} = \gamma(\phi_m - \chi) + (1 - \gamma)(E_q/q - \phi_0), \tag{3}$$

$$\phi_{Bn} = \gamma(\phi_m - \chi) + (1 - \gamma)(E_g/q - \phi_0), \qquad (3)$$

$$D_s = \frac{(1 - \gamma)\varepsilon_i}{\gamma\delta q^2}, \qquad (4)$$

where ϕ_{Bn} is the barrier height, ϕ_m is the metal work function, χ is the semiconductor electron affinity, E_g is the band gap of the semiconductor, ϕ_0 is the neutral level of the surface, ϵ_i is the dielectric constant of the interfacial layer, δ is the thickness of the layer, and D_S is the density of interface states. From the linear fits to the experimental data in Fig. 2, γ values were found to be 0.296 for the c-plane sample and 0.170 for the aplane one. Using these γ values, the densities of interface states D_S were estimated to be 2.59×10^{13} cm⁻²eV⁻¹ and 5.32×10^{13} cm⁻²eV⁻¹ for the c- and the a-plane sample, respectively. For this estimate, δ was assumed to be 5 Å (about 1 monolayer). Higher threading dislocation densities and basal stacking faults might increase the density of interface states for the a-plane GaN [16]. However, this does not exactly account for the result that c-plane GaN has a lower barrier height than a-plane GaN for the Ti Schottky contacts.

After depositing Pt, Au, and Ti metal layers on both c- and a-plane GaN, we performed XPS measurements to investigate the contact formation mechanisms in more detail. As shown in Fig. 3, the peak positions of Ga 3d and N 1s core levels shifted to higher binding energy as the metal work function decreased, which indicates that

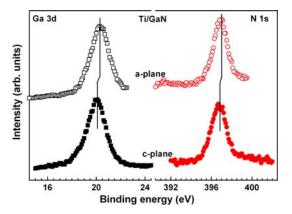


Fig. 4. (Color online) XPS spectra of Ga 3d and N 1s core levels for the Ti contacts to c- and a-plane n-type GaN.

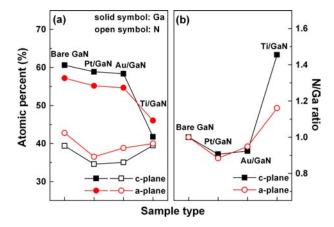


Fig. 5. (Color online) (a) Atomic percents of Ga and N atoms and (b) N/Ga ratio for the bare GaN, Pt/GaN, Au/GaN, and Ti/GaN samples obtained from XPS measurements.

the surface Fermi energy moved toward the conduction band edge, lowering the barrier height. Figure 4 depicts the peak positions of Ga 3d and N 1s core levels for the Ti/GaN contacts. The peak positions of the Ga 3d core level were found to be 20.0 (± 0.1) and 20.2 (± 0.1) eV for c- and a-plane GaN, respectively. Likewise, the peak positions of the N 1s core level were estimated to be 396.7 (± 0.1) and 396.8 (± 0.1) eV for c- and a-plane GaN, respectively. Likewise, the binding energy of a-plane GaN was found to be higher than that of c-plane GaN for the Pt and the Au contacts. These results imply that a-plane GaN has a lower barrier height than c-plane GaN, consistent with the results of I-V measurements for the Pt and the Au Schottky contacts. In contrast, the results are inconsistent with the results of I-V measurements for the Ti Schottky contacts.

Figure 5(a) shows that atomic percents of Ga and N atoms for the Pt and the Au contacts did not change significantly compared to those for the bare GaN samples. Thus, the effect of N vacancies on the barrier height will be marginal. The atomic percent of N atoms in the Ti contacts did not change much, but that of Ga atoms

decreased significantly for both the c- and the a-plane samples, which indicates the generation of Ga vacancies near the interface due to the out-diffusion of Ga atoms. The relative N/Ga ratio was evaluated by integrating the XPS spectra of the Ga 3d and the N 1s core levels (Fig. 5(b)). Here, the ratio of bare GaN samples was set to unity as a reference. The calculated N/Ga ratios in the c-plane GaN were 0.91, 0.92, and 1.45 for the Pt, Au, and Ti contacts, respectively. Likewise, the ratios in the a-plane GaN were 0.88, 0.95, and 1.16 for the Pt, Au, and Ti contacts, respectively. Based on these results, we can deduce that N vacancies for the Pt and the Au contacts and Ga vacancies for the Ti contacts were generated. The N vacancies acting as shallow donors [17] will increase the electron concentration near the interface and decrease the effective barrier height. On the other hand, the electrons near the interface will be annihilated by the compensation with Ga vacancies acting as deep acceptors [18], resulting in an increase in the effective barrier height. The analyses suggest that c-plane GaN has a higher barrier height than a-plane GaN for the Ti Schottky contacts, inconsistent again with the results of I-V measurements.

Using XPS measurements, Dumont et al. found that the Ti/GaN contact has regions containing out-diffused Ga atoms near the interface, but Pt. Pd. and Au/GaN contacts have no significant interfacial reaction [19]. Recently, Zhao et al. investigated the role of Ga vacancies in the GaN Schottky barrier photodetectors. They found that Ga vacancies might enhance both the tunneling probability and the reverse leakage current, leading to a decrease in the effective barrier height [20]. Thus, we can speculate that in the Ti Schottky contacts relatively higher density of Ga vacancies for the c-plane GaN enhances both the tunneling and the reverse leakage current, reducing the barrier height. Although further investigation is needed to explain the different out-diffusion rates of Ga atoms for c- and a-plane GaN, our results suggest that the role of Ga vacancies should be understood thoroughly to fabricate high-quality Ti-based contacts to n-type GaN.

IV. CONCLUSION

We investigated the electrical properties of Schottky contacts to c- and a-plane n-type GaN with Pt, Au, and Ti metals. We observed that the barrier heights of c-plane GaN were higher than those of a-plane GaN for the Pt and the Au Schottky contacts. In contrast, the barrier height of c-plane GaN was lower than that of a-plane GaN for the Ti Schottky contacts. Analyses based on the XPS spectra showed that c-plane GaN induced more Ga vacancies than a-plane GaN for the Ti Schottky contacts, which enhanced both the tunneling probability and the reverse leakage current, reducing the effective barrier height.

ACKNOWLEDGMENTS

This work was supported in part by the Basic Science Research Program (2010-0003594) through the National Research Foundation of Korea funded by the Ministry of Education, Science and Technology (MEST). XPS measurements were carried out in the Center for Research Facilities at Chungnam National University.

REFERENCES

- [1] S. Nakamura and G. Fasol, *The Blue Laser Diode* (Springer, Berlin, 1997).
- [2] T. Takeuchi, S. Sota, M. Katsuragawa, M. Komori, H. Takeuchi, H. Amano and I. Akasaki, Jpn. J. Appl. Phys. 36, L382 (1997).
- [3] F. Bernardini, V. Fiorentini and D. Vanderbilt, Phys. Rev. B 56, R10024 (1997).
- [4] E. T. Yu, G. Sullivan, P. Asbeck, C. Wang, D. Qiao and S. Lau, Appl. Phys. Lett. 71, 2794 (1997).
- [5] C. Chen, A. Vdivarahan, J. Yang, M. Shatalov, E. Kuokstis and M. Khan, Jpn. J. Appl. Phys. 42, L1039 (2003).
- [6] K. Matocha, V. Tilak and G. Dunne, Appl. Phys. Lett. 90, 123511 (2007).
- [7] X. Ni, Ü. Özgür, Y. Fu, N. Biyikli, J. Xie, A. Baski, H. Morkoç and Z. Liliental-Weber, Appl. Phys. Lett. 89, 262105 (2006).
- [8] V. Adivarahan, C. Chen, J. Yang, M. Gaevski, M. Shatalov, G. Simin and M. Khan, Jpn. J. Appl. Phys. 42, L1136 (2003).
- [9] H. Kim, S. Lee, Y. Park, J. Kwak and T. Seong, Appl. Phys. Lett. 93, 032105 (2008).
- [10] S. Phark, H. Kim, K. Song, P. Kang, H. Shin and D. Kim, J. Phys. D: Appl. Phys. 43, 165102 (2010).
- [11] K. Baik, Y. Seo, J. Kim, S. Hwang, W. Lim, C. Chang, S. Pearton, F. Ren and S. Jang, J. Phys. D: Appl. Phys. 43, 295102 (2010).
- [12] J. Law, E. T. Yu, B. Haskell, P. Fini, S. Nakamura, J. S. Speck and S. P. DenBaars, J. Appl. Phys. 103, 014305 (2008).
- [13] T. Mori, T. Kozawa, T. Ohwaki, Y. Taga, S. Nagai, S. Yamasaki, S. Asami, N. Shibata and M. Koike, Appl. Phys. Lett. 69, 3537 (1996).
- [14] S. Strite and H. Morkoç, J. Vac. Sci. Technol., B 10, 1237 (1992).
- [15] E. H. Rhoderick and R. H. Williams, Metal-Semiconductor Contacts (Oxford University press, London, 1988).
- [16] M. D. Craven, S. H. Lim, F. Wu, J. S. Speck and S. P. DenBaars, Appl. Phys. Lett. 81, 469 (2002).
- [17] J. Neugebauer and C. G. Van de Walle, Phys. Rev. B 50, 8067 (1994).
- [18] J. Neugebauer and C. G. Van de Walle, Appl. Phys. Lett. 69, 503 (1996).
- [19] J. Dumont, E. Monroy, E. Munoz, R. Caudano and R. Sporken, J. Cryst. Growth 230, 558 (2001).
- [20] D. Zhao, S. Zhang, W. Liu, X. Hao, D. Jiang, J. Zhu, Z. Liu, H. Wang, S. Zhang, H. Yang and L. Wei, Chin. Phys. B 19, 057802 (2010).