Effect of crystal orientation on ohmic contact formation for n-type gallium nitride

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Abstract. The present paper describes the influence of surface orientation of n-type GaN on the electrical properties and the interfacial reaction between GaN and Ti during annealing. Although the contact formed on (0001) Ga-face of GaN performs the highest electrical conductance in the as-deposited state, the conductance deteriorates significantly by annealing even at a low temperature of 773 K. A considerable amount of Ti-Ga intermetallic compounds is formed at the deteriorated interfaces, to which the deterioration is attributed.

1. Introduction

Gallium nitride (GaN) is commonly applied in light-emitting and laser diodes [1]. GaN has also a breakthrough potential for high-frequency-operated power electronic devices [2]. These applications require low-resistance ohmic contacts at interfaces between the GaN and the metallic circuits. To form low-resistance ohmic contacts on GaN, it is necessary to reduce the height and/or width of the Schottky barrier. In the case of n-type GaN, the work function of the contact material has to be shallower than the conduction-band edge of GaN, which is 4.11 eV below the vacuum level [3]. TiN is known as one of those contact materials because it has a sufficiently shallow work function of 3.74 eV [3]. On the other hand, to decrease the thickness of the Schottky barrier, it is effective to increase the carrier density in the GaN just under the contact material, which can be accomplished by implantation of dopants. The formation of TiN by interfacial reaction between GaN and Ti generates nitrogen vacancies (V\textsubscript{N}) in GaN, which work as donors at an energy level close to the conduction-band edge of GaN [4]. Therefore, it is preferable to form TiN on GaN by interfacial reaction between GaN and multilayered metallic film containing a Ti layer [5-8]. Furthermore, Maeda et al. have reported that V\textsubscript{N} formed in the sub-interface of GaN play the dominant role in developing ohmic properties, instead of the formation of TiN adjacent to GaN [9].

The (0001) Ga-face of GaN has been used in most of the papers reporting ohmic contact formation. This is due to the restriction in the growth of GaN single-crystals, which are generally epitaxially grown on sapphire substrates by metal-organic chemical vapor deposition. Recently, some techniques to produce free-standing bulk GaN single-crystals have been developed [10, 11]. Although they are still not the mainstream of mass production, the quality and size of the single-crystals will be rapidly improved. Thus, GaN single-crystals with other surface orientations will soon be available. On the other hand, it has not been clarified whether or not the (0001) plane is the best orientation for
achieving low-resistance conduction in the sheet and at the contact interface. Therefore, the electrical properties of the contacts on some representative surface orientations of GaN have to be compared.

The present study compares the electrical properties of GaN/Ti contacts formed on four different surface orientations of GaN: (0001) Ga-face, (000T) N-face, (01T0), and (1120).

2. Experimental procedure

Four kinds of free-standing n-type GaN substrates with surface orientations of (0001) Ga-face, (000T) N-face, (10T0), and (1120), respectively, were used. Hereinafter, the substrates are denoted by their surface orientations. A Ti layer was deposited on two separate areas with a 1.0 mm space between them on each substrate by radio-frequency (RF) magnetron sputtering. The substrates were fixed in the deposition chamber using 1.0-mm-wide Al ribbon masks. After evacuation of the chamber to 4.0×10⁻⁵ Pa, high-purity Ar of 8.0 Pa was introduced as the discharging gas. At first, the surfaces of the target and the substrates were sputter-cleaned consecutively. The RF power for sputter-cleaning of both the target and the substrates was 200 W. The sputter-cleaning time for the target was set at 600 s, whereas that for the substrates was set at 300 s. Finally, a layer of Ti was deposited under the RF power of 200 W and a deposition time of 600 s. The samples were annealed in a vacuum of 1.2×10⁻³ Pa. The annealing temperature was varied from 773 to 973 K. The samples were immediately cooled down in a vacuum furnace after reaching the target temperature, i.e., the samples were kept at the annealing temperature for a very short time (hereinafter the time is described as 0 s). Some of the samples were annealed at 973 K for 300 s in order to investigate the interfacial reaction behavior between GaN and Ti.

The interfacial structures were analyzed by X-ray diffraction (XRD) and transmission electron microscopy (TEM). Direct-current (DC) electrical conductivity was measured at 273 K by probing between the two Ti contacts separated by a distance of 1.0 mm formed on each sample.

3. Results and discussion

Figure 1 shows the DC current-voltage (I-V) profiles of as-deposited GaN/Ti contacts formed on the (0001), (000T), (1010), and (1120) surfaces of GaN. Two important features appear in the figure. One is that the profiles of all the contacts show a linear I-V relation, indicating that all contacts are ohmic in the as-deposited state. Therefore, the electrical conductance of each sample is obtained as a single value from the gradient of each line. The I-V relation remains linear after annealing. The other feature is that the conductance changes depending on the surface orientation of GaN. The highest
conductance is obtained with the contact on (0001). On the other hand, the conductance of the contacts formed on the other three surface orientations of GaN appears similar, as shown in the left part of Figure 2. The conductance of the samples changes depending on the annealing temperature and time. The change behavior of the contacts on (0001) appears different from that of the contacts on all other surface orientations. Although the highest conductance is obtained with the contacts on (0001) in the as-deposited state, the conductance deteriorates significantly by annealing even at a low temperature of 773 K for a very short time, and it becomes worse by annealing at higher temperatures. On the other hand, the conductance of the contacts on all other surface orientations of GaN is improved at first by annealing, and the improvement becomes larger by annealing at a higher temperature. However, the conductance of these samples decreases upon extending the annealing time to 300 s at 973 K.

It is likely that the conductance is improved owing to the formation of $V_N$ in the GaN sub-interface by interfacial reaction between GaN and Ti [9]. On the other hand, the deterioration could be caused by excessive reactions that form byproduct phases such as Ti-Ga compounds [12]. Thus, the deterioration of the conductance of the contacts is considered to be due to the transition from the interfacial reaction forming $V_N$ in GaN to that forming Ti-Ga compounds at the interface. The transition starts earlier and at a lower temperature in the contacts formed on (0001) than in those formed on other surface orientations.

![Figure 2. Changes in electrical conductance after annealing under various conditions.](image1)

![Figure 3. XRD patterns of the contact samples formed on (a) (1120), (b) (10\overline{1}0), (c) (0001), and (d) (0001) after annealing at 973 K for 300 s.](image2)
Figure 3 shows the XRD patterns of the contact samples after annealing at 973 K for 300 s. In the patterns of the samples formed on the (0001), (0 1 1 0), and (0 2 1 1) surfaces of GaN, peaks of GaN, Ti$_2$N, and Ti$_2$Ga$_3$ are identified, whereas GaN and Ti$_3$Ga$_5$ appear in the pattern of the sample formed on (1 0 0 0). Particularly, the peaks of Ti$_2$Ga$_3$ appearing in the pattern of the contact on (0001) are very strong, indicating that a considerable amount of Ti$_2$Ga$_3$ is formed at the interface. These results confirm the formation of Ti-Ga compounds at the interfaces with deteriorated electrical conductance. In addition, the reaction forming Ti-Ga compounds on the (0001) surface proceeds faster than that on the other surfaces of GaN.

Figure 4 shows a cross-sectional structure of the contact interface formed on the (0001) surface by annealing at 973 K for 300 s. In the bright-field image shown in Figure 4(a), a 60-nm-thick layer is formed adjacent to GaN by the interfacial reaction. The layer has a polycrystalline structure which consists of equiaxial grains. The electron diffraction pattern (EDP) corresponding to this area is shown in Figure 4(b) with some indices of diffraction spots. The EDP consists of a $[1210]$ zone axis net pattern of GaN [13] and randomly oriented spots from Ti$_2$N [14] and Ti$_3$Ga$_5$ [15]. The dark-field image of the same area using the Ti$_3$Ga$_5$ (321) diffraction is shown in Figure 4(c). Some grains in the layer adjacent to GaN appear bright, proving that the layer is Ti$_3$Ga$_5$. This result suggests that the interfacial reaction forming V$_N$ in GaN changes to that forming Ti-Ga compounds, i.e., from a donor-eliminating to a donor-forming reaction by excessive annealing. Therefore, the interfacial reaction has to be controlled to prevent the latter reaction in order to obtain a favorable ohmic interface.

4. Conclusions
Ti-based contacts were formed on four representative crystal surfaces of n-type GaN by deposition of Ti and subsequent annealing under various conditions to investigate the differences in the electrical properties and interfacial structure among the contacts on the four surfaces of GaN. The following points became clear: (1) The behavior of electrical conductance by annealing appears different between the contacts on the (0001) Ga-face and those on the other three surface orientations of GaN. The contacts on the
Ga-face exhibit the highest conductance in the as-deposited state. However, the conductance deteriorates by annealing even at a low temperature of 773 K for a very short time. On the other hand, the conductance of the contacts on the other three surfaces improves at first and then deteriorates with annealing.

(2) The deterioration of the electrical conductance of the contacts is attributed to the formation of Ti-Ga intermetallic compounds adjacent to GaN.

(3) The surface orientation of GaN affects the rate and the incubation time of the interfacial reaction to form Ti-Ga compounds. Consequently, the annealing condition for the contact formation has to be determined by taking the anisotropy of the reaction rate into account.

References
[1] Akasaki I 2007 J. Cryst. Growth 300 2
[2] Asif Khan M, Chen Q, Shur M S, Dermott B T, Higgins J A, Burm J, Schaff W J and Eastman L F 1997 Sol.-Stat. Electron. 41 1555
[3] Mohammad S N 2004 J. Appl. Phys. 95 7940
[4] Look D C, Reynolds D C, Hemsly J W, Sizelove J R, Jones R L and Molnar R J 1997 Phys. Rev. Lett. 79 2273
[5] Luther B P, Mohney S E and Jackson T N 1998 Semicond. Sci. Technol. 13 1322
[6] Fan Z, Mohammad S N, Kim W, Aktas Ö, Botchkarev A E and Morkoç H 1996 Appl. Phys. Lett. 68 1672
[7] Smith L L, Davis R F, Liu R J, Kim M J, and Carpenter R W 1999 J. Mater. Res. 14 1032
[8] Maeda M and Takahashi Y 2013 Int. J. Nanotechnol. 10 89
[9] Maeda M, Yamasaki T, and Takahashi Y, 2012 J. Phys. Conf. Ser. 379 012020
[10] Motoki M, Okahisa T, Nakahata S, Matsumoto N, Kimura H, Kasai H, Takemoto K, Uematsu K, Ueno M, Kumagay K, Koukitu A and Seki H 2002 J. Cryst. Growth 237-239 912
[11] Mori Y, Imade M, Murakami K, Takawasa H, Imabayashi H, Todoroki Y, Kitamoto K, Maruyama M, Yoshimura M, Kitaoka Y and Sasaki T 2012 J. Cryst. Growth 350 72
[12] Kimura K, Maeda M, and Takahashi Y 2013 Mater. Trans. 54 895
[13] Powder Diffraction Files (Newtown Square, PA: ICDD) 50-792
[14] Powder Diffraction Files (Newtown Square, PA: ICDD) 23-1455
[15] Powder Diffraction Files (Newtown Square, PA: ICDD) 42-811