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Comparative Study of Schottky Diode Characteristics in Ni, Ta and Ni/Ta Metal Contact Schemes on n-GaN

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We have reported current–voltage characteristics of Ta/- and Ni/Ta/n-GaN Schottky diodes under various thermal treatments. Experimental data indicate that the electrical characteristics of Ni/Ta diodes are controlled by the interfacial properties of the Ta and GaN heterointerface for the as-deposited samples and strongly affected by the presence of an oxide layer (Ta_2O_5) in those high-temperature-annealed diodes. In regard to Ta/Ni diodes, probably because of thermal stability and wide-band-gap properties of tantalum oxide, dramatic improvement in Schottky diode performance was resulted after annealing at high temperatures. The corresponding barrier height and ideality factor values can reach 1.17 eV and 1.09, respectively, even at an annealing temperature of 800°C.

KEYWORDS: Ni/Ta/n-GaN,Ta_2O_5

Because of the features of a direct band gap and wide wavelength tunability, GaN and related semiconductors have recently received much attention in terms of the fabrication of light-emitting devices, such as light-emitting diodes and laser diodes,[1–3] operating in green-, blue- and ultraviolet-wavelength regions. These compounds also possess properties of high thermal conductivity, high electron saturation velocity, excellent thermal stability, and resistance to chemical attack, making them nearly ideal materials in high-temperature and high-power electronic device applications. Up to now, the formation of high-quality and reliable barrier height was one of the most essential prerequisites for device development, particularly for operation in hostile environments. Experimental results have shown that a number of methods, including incorporation of a heavily doped layer, oxide interface, intermetallic film contact scheme, and other wide-band gap semiconductors in the device can effectively improve its Schottky properties.[4] However, probably due to the lack of studies, relatively few literary results have been addressed on this issue regarding the GaN material. Up-to-date, high-work-function metals, such as Pd (5.12 eV), Pt (5.65 eV), Au (5.1 eV), and Ni (5.17 eV) are customarily employed with most nitride groups in the fabrication of n-type GaN Schottky diodes. Indeed, a barrier height of 1 eV or greater can be achieved without difficulty. However, by reason of their reactive nature, these metals are unstable in terms of temperature.[5–8] They often react with the substrate at low temperatures, forming complex phases at the metal-semiconductor interface, and lead to degradation of device performance. In this paper, we propose an alternative way to enhance the GaN Schottky barrier height using Ni/Ta bilayer metal films. Our results indicate that when the Ni/Ta GaN diode is subjected to high-temperature annealing, fairly good GaN Schottky diode performance can be obtained.

The n-GaN film employed here was prepared using metalorganic vapor phase epitaxy. The corresponding film thickness is approximately 2 μm and the Hall concentration and electron mobility are 1.7×10^{17} cm^{-3} and 566 cm^2/V·s, respectively, indicating good GaN epilayer quality. To fabricate Schottky diodes, a large-area ohmic contact consisting of Ti/Al/Ni/Au was first deposited on the sample surface using an electron beam coater, which was subsequently thermally annealed at 600°C for 1 min in order to ensure good ohmic characteristics. Schottky contacts of 150 μm diameter with three different thicknesses of Ni/Ta metal contacts (20/20, 50/50, and 80 nm/80 nm) were made by sequentially evaporating Ta and Ni on the GaN substrate. These samples were then annealed in a quartz furnace with flowing nitrogen at various temperatures for 5 min. The resulting diode current–voltage (I–V) characteristics were measured using an HP4145B semiconductor parameter analyzer at room temperature. The effective barrier height and ideality factor are deduced from I–V measurement assuming the results can be described by the standard thermionic-emission equation. In attempt to gain a better understanding of the transport properties of the Ni/Ta/GaN Schottky diode with respect to thermal annealing, the results of pure Ni (40 nm) and pure Ta (40 nm) Schottky diodes obtained under similar experimental processes were also included in this study.

Prior to the discussion of the Schottky behavior of the Ni/Ta diode, we first present in Fig. 1 the results of pure Ni and pure Ta diodes annealed at various temperatures for 5 min, including the as-deposited samples. The corresponding Schot-

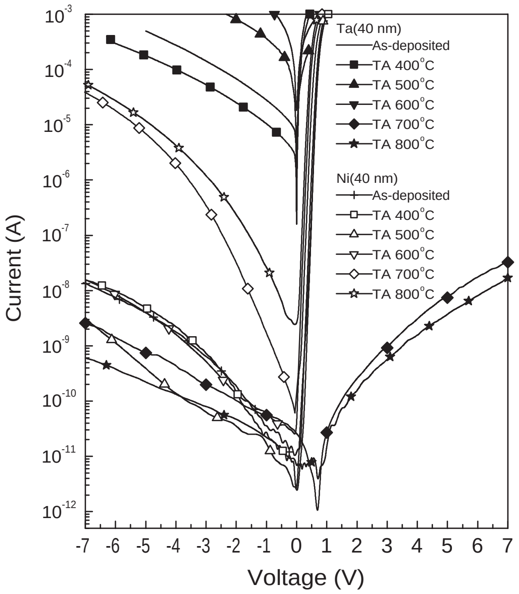

Fig. 1. I–V characteristics of Ni and Ta Schottky contact on n-GaN annealed at various temperatures from 400 to 800°C for 5 min.

Table I. Electrical parameters of Ni/ and Ta/n-GaN diodes.

Annealing temperature	Ni(40 nm)		Ta (40 nm)	
	Φ_b (eV)	n	Φ_b (eV)	n
As-deposited	0.90	1.17	0.41	1.17
400°C/5 min	0.91	1.15	0.48	1.17
500°C/5 min	0.93	1.14	—	—
600°C/5 min	0.85	1.20	—	—
700°C/5 min	0.76	1.21	Insulator-like	Insulator-like
800°C/5 min	0.70	1.21	Insulator-like	Insulator-like

— : denotes poor rectifying characteristics of diode

tky barrier height Φ_b and ideality factor n derived from the thermionic emission model are summarized in Table I. For the Ni diode, the tendency of its I–V characteristics with annealing temperature is basically similar to results published previously by other groups.[6] Good Schottky characteristics were observed for the as-deposited sample. The Φ_b and n are determined to be 0.90 eV and 1.17, respectively. They improve continuously with increasing annealing temperature up to 500°C, above which they deteriorate significantly to 0.85 eV and 1.20 at 600°C, 0.76 eV and 1.21 at 700°C, and 0.7 eV and 1.21 at 800°C. Liu *et al.*,[6] Bermudez and Kaplan[7] and Venugopalan *et al.*[10] doubt that such degradation could attribute greatly to the dissolution of Ga into the Ni film and a burst loss of N in GaN when the annealing temperature is elevated to above 600°C. We believe this is also the case observed in our Ni/GaN diodes.

In contrast to Ni, very unlikely behavior was observed for the Ta/GaN diode. For the as-deposited sample, the values of Φ_b and n are 0.41 eV and 1.17, respectively. Although the barrier height is not sufficiently high, as expected from its low work function value, typical Schottky I–V characteristics can still be observed. When the diode is annealed, poorer quality results; the corresponding reverse current is increased, the barrier height is decreased and virtually ohmic characteristics are observed for the 600°C-annealed diode. Nonetheless, as shown in Fig. 1, a dramatic change occurs in the electrical behavior when the temperature is elevated to >700°C. The measured reverse current drops sharply to the range of 10^{-8} to 10^{-11} A, and, more interestingly, a nearly symmetric feature is observed at forward-biased voltage. Such a peculiar change in electrical properties with annealing temperature strongly suggests that a phase transformation occurs for Ta during the heat treatment at approximately 600–700°C.

It is worth mention that the observed results for the Ta/n-GaN Schottky diode at various annealing temperature are not exactly the same as those for Ta on conventional semiconductors, such as n-GaAs, as reported by Lahav and Eizenberg,[11,12] and Huang and Jean,[13] in which the Ta contact still preserves its ohmic characteristics at annealing temperatures above 650°C. Although we can ascribe this discrepancy partly to the substrate itself due to the fact that these is a larger kinetic barrier for the decomposition of GaN than that of GaAs,[14] we believe it also is due significantly to the various thermal treatment conditions employed in the experiments. Lahav and Eizenberg conducted annealing in a vacuum ambient, while we performed annealing in an open-tube furnace with continuous nitrogen gas flow, which cannot exclude completely the existence of residual oxygen in the system. As is known, Ta reacts easily with oxygen. It has been reported that the Ta metal in a similar environment will partially oxidize at a temperature of 400°C and convert entirely into Ta_2O_5 at 550°C. This also occurs in our samples.[15] Consequently, the high-temperature-annealed Ta/n-GaN diode no longer represents the original metal-semiconductor structure, but more closely resembles an insulator-semiconductor one. This argument could explain the observed insulator-like I–V characteristics of our high-temperature Ta/GaN films.

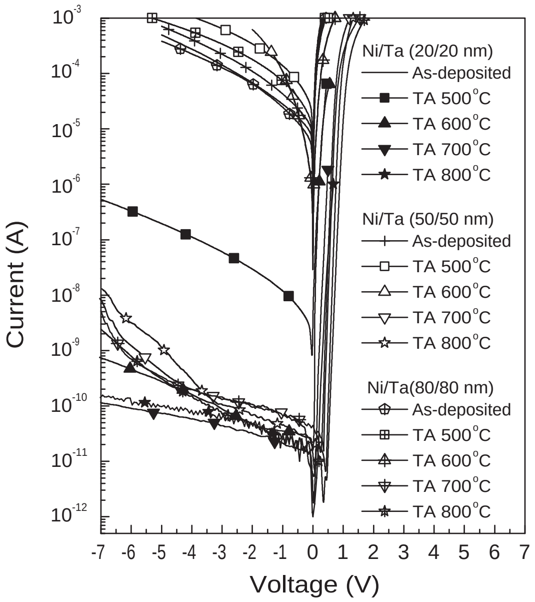

Fig. 2. I–V characteristics of Ni/Ta/n-GaN Schottky diodes annealed at various temperatures from 500 to 800°C for 5 min.

Finally, we focus our discussion on the cases of the Ni/Ta bilayer films. Figure 2 presents the semilog forward- and reverse-bias I–V characteristics of Ni/Ta/n-GaN Schottky diodes with thicknesses varying from 20/20, 50/50 to 80 nm/80 nm, thermally treated under the same conditions as described earlier. Again, the results of as-deposited samples are also presented in the figure. All of their device parameters are summarized in Table II. It is interesting to note that for the as-deposited Ni/Ta samples, regardless of film thickness, their barrier height and ideality factor values are not only similar (approximately 0.42 eV and 1.18, respectively), but also very close to those of the pure as-deposited Ta diode (0.41 eV and 1.17, respectively). For the as-deposited samples, the metallic compound adjacent to the GaN substrate is unoxidized at this stage and is simply in the form of pure Ta metal itself, hence the carrier transport is determined primarily by the physical properties of Ta and GaN and the intermediate induced interface states. As a result, very similar electrical properties are observed for our as-deposited Ni/Ta/GaN and pure Ta/GaN diodes.

When the annealing temperature is elevated, the thin 20 nm/20 nm Ni/Ta diode shows a significant reduction in the reverse leakage current, accompanied by a notable increase in the Φ_b value. Its barrier height continues to increase to 0.92 eV at 700°C and 0.93 eV at 800°C, but the ideality factor begins to deteriorate considerably to 1.26 and 1.45, respectively. The fact that the ideality factor values are much larger than 1.2 indicates that the transport properties of the devices are not well described by thermionic emission. On the other hand, the I–V characteristics of the thicker Ni/Ta diodes re-

Table II. Electrical parameters of Ni/Ta/n-GaN diodes.

Annealing temperature	Ni/Ta (20/20 nm)		Ni/Ta (50/50 nm)		Ni/Ta (80/80 nm)	
	Φ_b (eV)	*n*	Φ_b (eV)	*n*	Φ_b (eV)	*n*
As-deposited	0.42	1.17	0.41	1.18	0.42	1.18
500°C/5 min	0.58	1.18	—	—	—	—
600°C/5 min	0.71	1.20	—	—	—	—
700°C/5 min	0.92	1.26	1.12	1.08	1.08	1.10
800°C/5 min	0.93	1.45	1.16	1.08	1.17	1.09

— : denotes poor rectifying characteristics of diode

main almost unchanged at annealing temperatures of 500 and 600°C as compared to the as-deposited samples. More interestingly, when the annealing temperature is increased to above 700°C, comparatively good diode performance can be obtained. This is very different from the cases of pure Ni/ and Ta/GaN diodes, where severe degradations are known to occur in this temperature region. Their values lie in the range of 1.08–1.17 eV for Φ_b and 1.08–1.10 for n, which are comparable to the best values ever reported for the n-type GaN Schottky diode without any thermal treatment.

We believe that the transport properties of the thermally annealed Ni/Ta/n-GaN Schottky diodes are closely related the extent of Ta oxidation, as confirmed by X-ray photoemission spectroscopy results in our previous paper.[15] That is the barrier height of the annealed Ni/Ta diode is no longer governed by pure Ta, but instead by the tantalum oxide. According to Robertson and Chen,[16] the tantalum oxide is more thermally stable than the pure Ni and Ta metals, and also has high expected barrier height values. Well-behaved Schottky diode performances therefore result for our high-temperature Ni/Ta/GaN diodes.

We have reported current–voltage characteristics of the Ta/GaN and Ni/Ta/GaN Schottky diodes. Experimental data indicate that the values of Schottky barrier height and ideality factor for the as-deposited samples are 0.41 eV and 1.17 for Ta/GaN, and approximately 0.42 eV and 1.18, respectively, for all of our Ni/Ta/GaN diodes. The similar rectifying characteristics of these Ni/Ta/GaN and Ta/GaN diodes strongly suggest that the as-deposited Ni/Ta/GaN diode performance is determined primarily by the interfacial properties of the Ta and GaN metal-semiconductor heterointerface. When these Schottky diodes are subjected to high-temperature annealing for 5 min, very different electrical behaviors result. Severe degradations are observed in both pure Ni and pure Ta diodes, while good Schottky diode performances can still be attained for the Ni/Ta/GaN diodes, particularly for the thicker ones. Such an improvement in Ni/Ta/GaN diodes with increasing temperature can be attributed greatly to the formation of a tantalum oxide layer, which makes the device behave more like a metal-insulator-semiconductor diode. Because the Ni/Ta_2O_5 interface exhibits a high barrier height, better Schottky properties are obtained for our Ni/Ta/GaN diodes.

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