AIP | Applied Physics Letters

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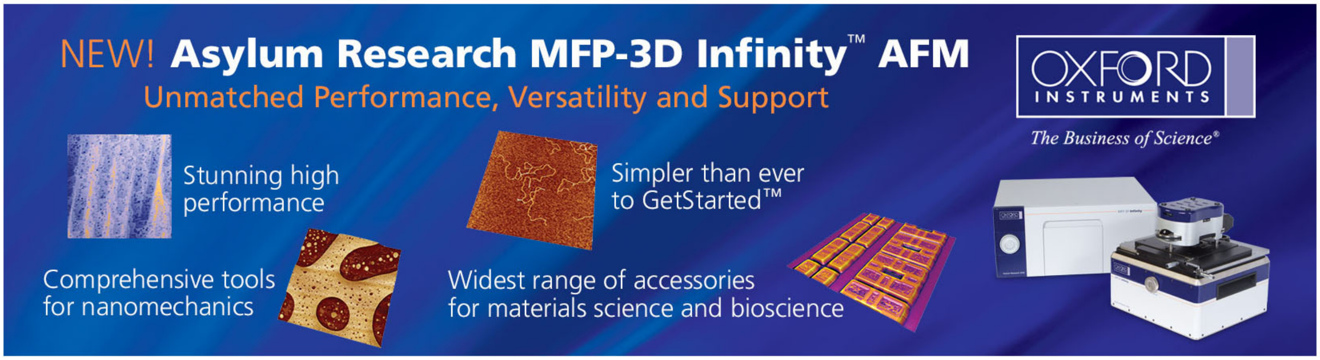
Citation: Applied Physics Letters **80**, 595 (2002); doi: 10.1063/1.1425455
View online: http://dx.doi.org/10.1063/1.1425455
View Table of Contents: http://scitation.aip.org/content/aip/journal/apl/80/4?ver=pdfcov
Published by the AIP Publishing



APPLIED PHYSICS LETTERS VOLUME 80, NUMBER 4 28 JANUARY 2002

Thermal stability study of Ni/Ta *n*-GaN Schottky contacts

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(Received 24 July 2001; accepted for publication 15 October 2001)

The Schottky behavior of Ni/Ta and Ni contacts on *n*-GaN was investigated under various annealing conditions by current–voltage measurements. It is found that with the addition of Ta between the Ni layer and the GaN substrate the thermal stability properties of devices can be significantly improved. Experimental results indicate that a high quality Ni/Ta *n*-GaN Schottky diode with an ideality factor and barrier height of 1.16 and 1.24 eV, respectively, can be obtained under 1 h annealing, at 700 °C.
[DOI: 10.1063/1.1425455]

Due to the properties of wide band gap, high electron saturation velocity, large breakdown field and thermal stability GaN materials have recently attracted much attention in the area of high-temperature, high-power device applications,[1–3] such as metal–semiconductor field effect transistors and high electron mobility transistors. However, the realization of these devices not only counts on the quality of the material properties, but also relies critically on the performance of metal contacts, in particular the Schottky contacts. Therefore, the exploration of thermally stable Schottky contacts is very desirable for implementation of such kinds of devices. With regard to a GaN Schottky study, numbers of elemental metals, including Pd, Pt, Ti, Ni, Au, Cr and Re,[4–8] and intermetallics of PtSi and NiSi have been investigated extensively and several advancements have been achieved.[8–9] Here, we present an alternative method that uses a Ni/Ta contact scheme to improve the thermal stability properties of the GaN Schottky contact. We observed that a high quality Schottky diode with an ideality factor and barrier height of 1.16 and 1.24 eV, respectively, can be obtained for samples annealed under severe annealing conditions of 700 °C for 1 h.

The 2-μm-thick n-GaN film employed here was prepared using metalorganic vapor phase epitaxy. The corresponding background concentration and electron mobility are $1.7 \times 10^{17}\,\mathrm{cm}^{-3}$ and $566\,\mathrm{cm}^2/\mathrm{V}\cdot\mathrm{s}$, respectively. In order to characterize electrical properties, Ni/Ta Schottky diodes were then made for these samples.

In Figs. 1 and 2, we present the dependence of the forward and reverse bias characteristics of pure Ni and Ni/Ta bilayer Schottky contacts on *n*-GaN annealed at various temperatures from 500 to 800 °C from 5 min to 1 h, respectively. From the forward log $I-V$ curves, the ideality factors n, Schottky barrier heights ϕ_b, and saturation current I_s of these diodes can be obtained. The extracted device parameters for these Schottky diodes are summarized in Table I.

As far as the Ni/n-GaN Schottky diodes are concerned, under a fixed annealing time of 5 min we find that the forward $I-V$ curve (open symbols) tends to shift to the left (low voltage and high current) with an increase in temperature, indicating poorer rectifying characteristics have occurred in these high-temperature annealed Ni diodes. Clearer pictures can be seen from the deduced device parameters. As can be seen in Table I, despite the fact that a good quality Schottky diode with an ideality factor of 1.14 and barrier height of 0.93 eV can be obtained at an annealing temperature of 500 °C, a further increase in the annealing temperature does deteriorate the $I-V$ characteristics, particularly that of the barrier height. It changes to 0.85 eV at 600 °C, 0.76 eV at 700 °C, and 0.70 eV at 800 °C. Such degradation is attributable primarily to the onset of interface reactions of Ni and GaN and a burst of loss of N at the interface at 550–600 °C,

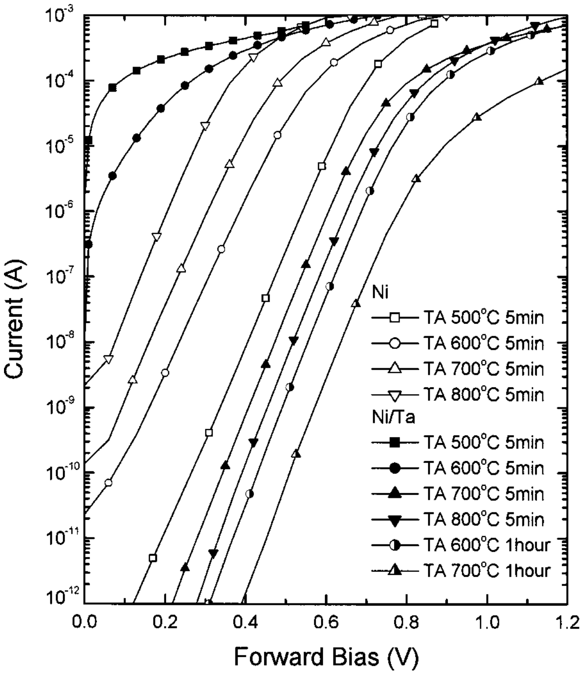

FIG. 1. Forward $I-V$ characteristics of Ni and Ni/Ta n-GaN Schottky contacts after being annealed at temperatures from 500 to 800 °C for 5 min or 1 h, respectively.

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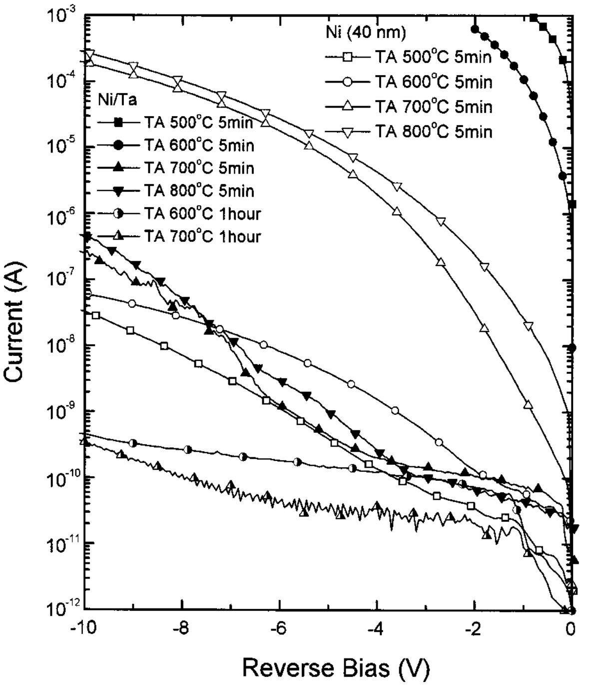

FIG. 2. Reverse $I-V$ characteristics of Ni and Ni/Ta n-GaN Schottky contacts after being annealed at temperatures from 500 to 800 °C for 5 min or 1 h, respectively.

in accord with the arguments given by Liu *et al.*,[9] by Bermudez and Kaplan,[10] and by Venugopalan *et al.*[11]

In contrast, very unlike behavior is observed in the Ni/Ta n-GaN Schottky diodes after annealing at various high temperatures for 5 min. As can be seen in Fig. 1, when Ta is added to the contact layer the corresponding forward $I-V$ curve (closed symbols) tends to shift to the right with an increase in annealing temperature, rather than the tendency to shift to the left in the Ni-only diodes. Moreover, it is worth mentioning that the Ni/Ta Schottky diode displays virtually no rectifying characteristics at annealing temperatures of 500–600 °C. It improves almost immediately after the temperature exceeds 700 °C. The resultant ideality factor n is almost close to 1 and the barrier heights are 1.12 and 1.16 eV, respectively, for 700 and 800 °C samples. Such good Schottky characteristics are unusual for high-temperature annealed GaN diodes.

To examine the long-term thermal stability of the Ni/Ta GaN Schottky diode, we conducted further experiments with an extended annealing time of 1 h at 600 and 700 °C, respectively, and of 30 min at 800 °C. The results are also shown in Figs. 1 and 2 and in Table II. It is interesting to note that no clear evidence of degradation is observed for 600 and 700 °C annealed diodes under prolonged thermal treatment. In fact, slightly better results are obtained for these diodes. The corresponding ideality factor remains almost unchanged, but the barrier height improves from 1.12 to 1.17 eV for 600 °C and 1.16–1.24 eV for 700 °C as the annealing time is increased from 5 min to 1 h. As for the 800 °C sample, insulator-like behavior is observed for an annealing time of 30 min.

For thermal stability study of GaN, it has been demonstrated that both conventional Pt and N GaN Schottky diodes,[8,9] can be stable up to 400–500 °C for 1 h annealing, as shown in Table II. The addition of Si to the Pt GaN diode is found to have a noticeable effect in improving the thermal stability compared to the Pt-only diode, for which the annealing temperature can be increased up to 600 °C for 1 h without severe degradation of its performance. Although Venugopalan and Mohney[6] in their study have shown that a Re contact is more thermal stable than most reported GaN Schottky contacts, satisfactory rectifying characteristics can only be obtained at an operating temperature as high as 150 °C. Based on the above discussions, we determine that our Ni/Ta/n-GaN does perform comparatively well with regard to the thermal stability since a high quality Schottky diode with a barrier height of 1.24 eV and an ideality factor of 1.16 can still be obtained at a temperature of 700 °C for less then 1 h annealing.

One additional point worth mentioning is that when the Ni/Ta GaN Schottky diode is subjected to long-term exposure, for example, 1 h, at 600 or 700 °C, the reverse leakage current is reduced to a value of 10^{-7} A/cm^2 and exhibits nearly voltage-independent characteristics. These findings together with the excellent forward characteristics seem to imply that the metal–semiconductor interface that results in this case is highly metallurgically stable and nearly free of any interface reactions and component interdiffusion (which will be discussed in more detail later) since, if imperfections do occur, they will form an intervening dipole layer and other contaminants at the interface and cause an increase in leakage current at high reverse bias voltage.

The strong dependence of electrical properties in the Ni/Ta/n-GaN Schottky diode on the annealing temperature

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

Metal	Annealing temperature (°C)	Ideality factor n	Barrier height, ϕ_b (eV)	Series resistance, R_s (Ω)	Leakage current, J_R (A/cm^2)
Ni	500, 5 min	1.14	0.93	200	1×10^{-6}
	600, 5 min	1.20	0.85	250	1×10^{-5}
	700, 5 min	1.21	0.76	250	1×10^{-2}
	800, 5 min	1.21	0.70	280	2.5×10^{-2}
Ni/Ta	500, 5 min		Poorly rectified		
	600, 5 min		Poorly rectified		
	700, 5 min	1.08	1.12	600	1.5×10^{-6}
	800, 5 min	1.08	1.16	950	1.5×10^{-6}
	600, 1 h	1.09	1.17	650	9.5×10^{-7}
	700, 1 h	1.09	1.24	3800	1×10^{-7}
	800, 30 min		Insulator like		

TABLE II. Comparison of Schottky properties of GaN diodes.

Metal	Ideality factor, n	Barrier height, ϕ_b ($I-V$) (eV)	Barrier height, ϕ_b ($C-V$) (eV)	Stable temperature (°C)	Reference
Ni (100 nm)	1.16	⋯	1.06	400, 5 min	7
Ni (100 nm)	1.10	0.88	1.09	500, 1 h	9
Pt	1.16	0.73	0.91	400, 1 h	8
Pd (200 nm)	1.04	0.94	1.07	300/5 min	4
Re (70 nm)	1.09[a]	0.78	1.03	700/10 min	6
Ni/Ga/Ni	⋯	⋯	⋯	700/10 min	11
NiSi (Ni/Si/Ni)	1.14	0.86	1.47	600/1 h	9
PtSi (Pt/Si/Ni)	1.12	0.69	0.74	600/1 h	8
Ni/Ta (50/50 nm)	1.09	1.17	⋯	700/1 h	This work

[a] Operation temperature of 150 °C.

and annealing time is believed to correlate closely to the degree of partial oxidation of the Ta metal layer, as confirmed by our Auger electron spectroscopy depth profile analysis and x-ray photoelectron spectroscopy measurements published in a previous paper.[12] The presence of oxygen in all of our samples except the as-deposited one clearly indicates that the oxygen originates primarily from the process environment during the thermal annealing step. For the experimental setup used here, we have found that the Ta film starts to oxidize at 400 °C and almost fully converts into tantalum oxide at 700 °C and above, particularly for long-term exposure. Thus, the evolution of electrical properties for the Ni/Ta/n-GaN diode on the annealing temperature can be inferred as follows. When the sample is annealed at low temperatures where the amount of unintentionally oxygen introduced into the contact region is still rather small, the Ta near the GaN remains in its elemental form. The resulting Ni/Ta/n-GaN film in this case behaves virtually the same with respect to the forward and reverse $I-V$ characteristics, i.e., nearly ohmic characteristics, as the Ta/n-GaN diode. On the other hand, when the oxidation of Ta is more complete, the Ni/Ta/n-GaN diode becomes more of a metal–insulator–semiconductor type structure and the effective barrier height in this case is determined largely by the physical parameters of the Ni and Ta_2O_5 layers and the GaN substrate, including the work function, electron affinity and Schottky barrier pinning factor S. By employing $S=0.4$,[13] the calculated barrier height for pure Ni on Ta_2O_5 is ~1.4 eV, very close to that of the observed maximum barrier height, 1.24 eV, in our Ni/Ta/n-GaN diodes. But if the diode is subjected to prolonged exposure at a higher temperature the tantalum oxide becomes too thick for the carriers to flow over and as a result insulator-like diode behavior is observed for our 800 °C GaN diode.

With regard to the thermal stability of these diodes, it is known that tantalum oxide possesses a relatively low Gibbs formation energy, $G(Ta_2O_5)=-484$ Kcal/mol, compared to $G(Ga_2O_3)=-260$, $G(Ta_2N)=-65$ and $G(\mathrm{GaN})=-26.4$ Kcal/mol,[14] and once the tantalum oxide has formed, the oxide–semiconductor interface becomes quite thermodynamically stable. It not only successfully stops the outdiffusion of Ga and N from the substrate, but also essentially prevents the penetration of Ni into GaN and accumulation on its surface to form metal gallides that will degrade the Schottky performance. Thus, the formation of a highly stable thin tantalum oxide layer between Ni and the GaN substrate may be the reason for the good thermal stability of our Ni/Ta/n-GaN diodes.

In summary, we have carried out an electrical study of a Ni/Ta/n-GaN Schottky diode under prolonged exposure at high temperatures. Our results indicate better Schottky performance can be obtained for an n-type GaN diode if an intermediate Ta layer is added between Ni and the GaN substrate. After high temperature annealing, the optimum ideality factor and barrier height can reach values of 1.08 and 1.24 eV, respectively. More important, it is found that high quality diode performance can still be obtained for these diodes under 700 °C, 1 h thermal annealing, which is unusual for an n-GaN Schottky diode. The above finding suggests a Ni/Ta Schottky contact is potentially useful for GaN high-temperature, high-power device applications.

The authors would like to acknowledge financial support from the National Science Council, Republic of China, under Contract Nos. NSC89-2212-M009-061 and -056.

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