Schottky barrier height of boride-based rectifying contacts to *p*-GaN

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Schottky contact formation on *p*-GaN using a W_2B-based metallization scheme was investigated using x-ray photoelectron spectroscopy (XPS), current-voltage (*I-V*), and capacitance-voltage (*C-V*) measurements. The Schottky barrier height (SBH) determined from XPS is 2.7 eV, whereas fitting of the *I-V*'s gives 1.2 and 3.8 eV depending on the assumed mechanism of forward current flow. While the *C-V*'s and the measurement temperature dependence of the *I-V*'s support tunneling as being the dominant transport mechanism, this latter approach overestimates the true SBH of W_2B/p-GaN contacts due to the presence of an interfacial layer acting as an additional barrier to carrier transport. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2357855]

An important aspect of the improvement of GaN-based devices for optoelectronics and high temperature/high power electronics is the development of more reliable and thermally stable Ohmic and Schottky contacts to both *n*-type and *p*-type GaN. In the case of *n*-GaN, while investigations of rectifying contacts with high work function metals such as Ni, W, Pd, Pt, and Au have revealed Schottky barrier heights (SBHs) in the 0.9–1.3 eV range,[1,2] annealing above ~500 °C usually greatly reduces the SBH to the point where the rectifying behavior disappears.[3–5] For *p*-GaN, higher SBHs are expected since the barrier heights for *n*-GaN and *p*-GaN should add up to the GaN band gap of 3.4 eV in the Schottky-Mott model.[6] However, there is a fairly large discrepancy in the reported SBH values for most metals on *p*-GaN, ranging from ~0.5 to 2.9 eV even for the same metallization scheme.[6–11] This essentially results from the fact that the mechanism of forward current flow is generally not clearly established, leading to several possible interpretations of the current-voltage (*I-V*) characteristics.

In this letter, we investigate the Schottky contact formation on *p*-GaN using a W_2B-based metallization scheme. Transition metal borides such as ZrB_2, TiB_2, CrB_2, W_2B_5, and W_2B are very promising for thermally stable contacts to GaN due to their high melting temperature and high thermodynamic stability. Recent works by Khanna *et al.*[12] and Oder *et al.*[13] have indeed reported improved thermal stability of boride-based Schottky contacts to *n*-GaN in comparison to more conventional metallurgies. While the forward-bias *I-V* characteristics for *n*-GaN rectifying diodes are usually well described using a thermionic emission (TE) model, interpretation of the *I-V*'s for *p*-GaN is much less straightforward. While some authors have reported accurate determination of the SBH using the TE model,[9] others have demonstrated the dominance of thermionic field emission (TFE).[7,8,10,11] Precise characterization of the boride-based rectifying contacts to *p*-GaN thus first required a detailed analysis of the carrier transport mechanism. To this end, we analyze in the following the SBH of W_2B-based Schottky contacts to *p*-GaN using *I-V*, capacitance-voltage (*C-V*), and x-ray photoelectron spectroscopy (XPS) measurements. Even though TFE is demonstrated to be the most dominant mechanism of forward current flow, this approach overestimates the true SBH of boride/*p*-GaN contacts due to the presence of an interfacial layer acting as an additional barrier to carrier transport.

The *p*-GaN samples under investigation were 1-μm-thick Mg-doped GaN layers grown by metal organic chemical vapor deposition on 1-μm-thick undoped buffers on *c*-plane Al_2O_3 substrates. The hole concentration obtained from Hall measurements after acceptor activation annealing was $\sim 10^{17}$ cm^{-3}. The surface was cleaned by sequential rinsing in acetone, ethanol, and 10:1 H_2O:HCl prior to insertion in the deposition chamber. W_2B(500 Å)/Pt(200 Å)/Au(800 Å) was used as the Schottky metallization scheme. Au was added to lower the contact sheet resistance while Pt is a diffusion barrier. All metals or compounds were deposited by Ar plasma-assisted rf sputtering at a pressure of 15 mTorr and rf powers of 250–400 W. The contacts were patterned by lift-off of lithographically defined photoresist and annealed at 500 °C for 1 min in a flowing N_2 ambient in a rapid thermal annealing furnace. For Ohmic contacts, we used Pt/Au annealed at 500 °C in O_2 for 30 s prior to deposition of the Schottky metallization. Ring contact geometry for the diodes was employed, with the Schottky contacts surrounded by the Ohmic contacts. The Schottky contact dots were 40 μm in diameter and the surrounding was 60 μm in inner diameter and 70 μm in outer diameter.

The *I-V*'s were recorded over the temperature range of 25–200 °C using a probe station and an Agilent 4145B parameter analyzer. Since it is not clear which mechanism governs current transport in *p*-GaN rectifying diodes, the SBH was extracted using both TE and TFE models. Ignoring SBH lowering due to image force, the current density under forward bias J_F for TE can be written as[15]

$$J_F = A^* T^2 \exp\left(-\frac{e\phi_B}{k_B T}\right)\exp\left(\frac{eV}{nk_B T}\right), \quad (1)$$

where $A^* = 103.8$ A cm^{-2} K^{-2} is the effective Richardson's constant for *p*-GaN,[14] T is the absolute temperature, e is the electronic charge, ϕ_B is the SBH, k_B is the Boltzmann's constant, and V is the applied voltage. In the presence of tunneling, J_F becomes[15]

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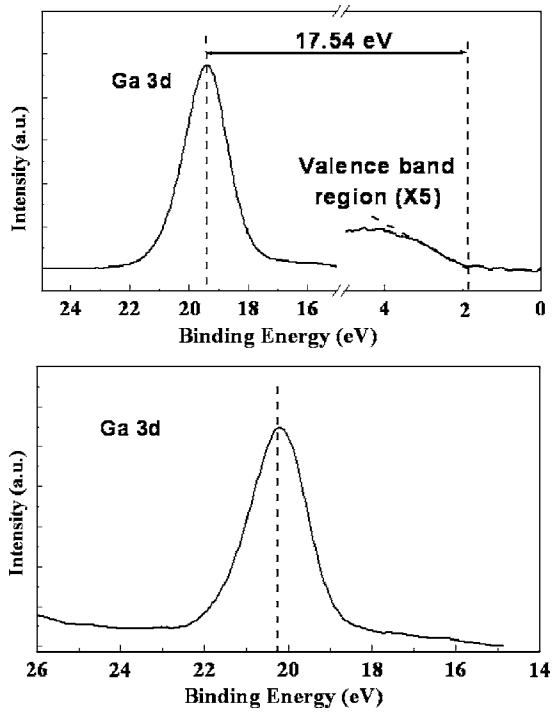

FIG. 1. XPS spectra without (top) and with (bottom) a boride-based overlayer. In the top figure, the left-hand spectrum corresponds to the Ga 3*d* core level, whereas the right-hand panel presents the spectrum of the valence band region.

$$J_F = J_0 \exp(eV/E_0), \tag{2}$$

where the saturation current density J_0 is given by

$$J_0 = \frac{A^*T[\pi E_{00}q(\phi_B - V - \xi)]^{0.5}}{k_B \cosh(E_{00}/k_BT)} \exp\left(-\frac{e\xi}{k_BT} - \frac{e(\phi_B - \xi)}{E_0}\right). \tag{3}$$

In Eq. (3), $\xi=(E_F\text{-}E_V)/e$ is the difference between the valence band maximum and the position of the Fermi level and $E_0=E_{00}\coth(E_{00}/k_BT)$ is the characteristic energy related to the tunneling probability. In this study, we assume $\xi=0.13$ V.[10,16] For *p*-GaN, $E_{00}(\text{eV}) \approx 7.75 \times 10^{-12}\sqrt{N_A(\text{cm}^{-3})}$,[7,10] N_A being the density of acceptors.

C-V measurements were performed using an Agilent 4284A precision *LCR* meter in the parallel mode. The modulation frequency was set to 1 kHz. The SBH was determined according to $\phi_B = V_{\text{int}} + E_A + (k_BT/q)\ln g$, where V_{int} is the extrapolated intercept voltage of the reverse bias in the $1/C^2$ vs *V* plot, $E_A \approx 0.12$ eV is the activation energy of Mg dopants in *p*-GaN, and $g=2$ is the degeneracy factor for acceptors.[17] Note that in our case, the series resistance ($\sim$2 kΩ) and the junction conductance ($\sim 10^{-8}$–10^{-9} S) were low enough so that the measured capacitance corresponds to the proper junction capacitance.

XPS measurements were taken with a Physical Electronics 5100LSci spectrometer with an aluminum x-ray source (energy of 1486.6 eV). Charge correction was performed by using the known position of the C-(C, H) line in the C 1*s* spectra at 284.8 eV. The SBH was determined from the binding energy of the Ga 3*d* core level E_B and the energy difference between that core level and the valence band maximum E_{VC} according to $\phi_B = E_B - E_{VC}$.[10,18]

Figure 1 presents an example of the Ga 3*d* core level and the valence band spectrum collected on a *p*-GaN surface without a W_2B overlayer. From this figure, we find $E_{VC}=17.54$ eV, which is in reasonable agreement with the value of 17.8 eV reported previously.[10,19] After W_2B deposition, Fig. 1 shows that the binding energy of the Ga 3*d* core level is $E_B=20.25$ eV, thereby yielding $\phi_B=2.71$ eV. This value is similar to the 2.68–2.78 eV values reported by Yu *et al.*[7] for Ni/*p*-GaN. For W_2B-based rectifying contacts to *n*-GaN, Khanna *et al.*[12] have reported $\phi_B \sim 0.55$ eV. Based on the Schottky-Mott model,[6] this suggests $\phi_B \sim 2.85$ eV for W_2B/*p*-GaN. Our result is only 5% lower than that predicted by this model.

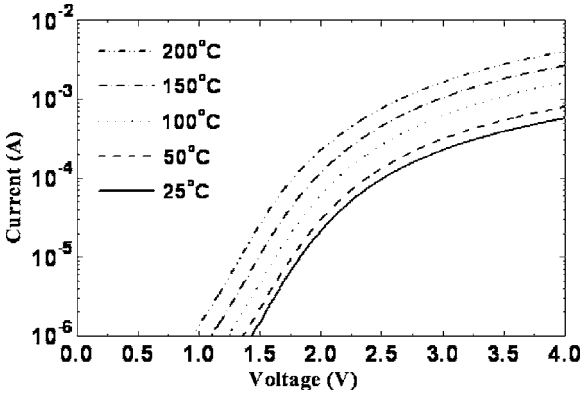

FIG. 2. Forward-bias current-voltage characteristic of Au/Pt/W_2B/*p*-GaN Schottky diodes as a function of measurement temperature.

The *I-V* characteristics as a function of the measurement temperature are shown in Fig. 2. All log *I* vs *V* curves measured between 25 and 200 °C exhibit a linear region at low forward bias (up to $\sim$2.0 V) and a less steep region at higher voltages. Furthermore, all log *I* vs *V* curves are parallel. As noted in Refs. 7, 8, 10, and 11 for *p*-GaN samples with relatively high doping levels ($>10^{17}$ cm^{-3}), this latter result is inconsistent with the TE model but typical for carrier transport with a dominant tunneling component. Note that Shiojima *et al.*[9] have reported accurate determination of the SBH using the TE model. However, the acceptor concentration in their *p*-GaN samples was relatively low ($\sim 10^{16}$ cm^{-3}). In our case, the characteristic energy related to the tunneling probability is 110 meV, which is about four times higher than the thermal energy (25 meV at 300 K). This result clearly supports tunneling as the most dominant mechanism of forward current flow. Nevertheless, this value of E_0 corresponds to an acceptor density of about 2×10^{20} cm^{-3}, which is higher than that expected from the Mg concentration alone ($\sim 10^{19}$ cm^{-3}). This can probably be attributed to the presence of acceptorlike deep level defects induced by the high Mg doping.[11,12] In such a case, tunneling can still be described by means of Eqs. (2) and (3) by redefining the parameter E_0 as the characteristic energy related to the probability for defect-assisted tunneling.[21]

Table I compares the SBH determined from XPS, *I-V* (TE and TFE), and *C-V* measurements. The value of ϕ_B obtained assuming tTFE (3.8 eV) is much higher than that cal-

TABLE I. Characteristics of W_2B-based rectifying contacts to *p*-GaN.

XPS	TE	TFE	*C-V*
ϕ_B=2.7 eV	ϕ_B=1.2 eV n=4.4	ϕ_B=3.8 eV E_0=110 meV	ϕ_B=4.1 eV

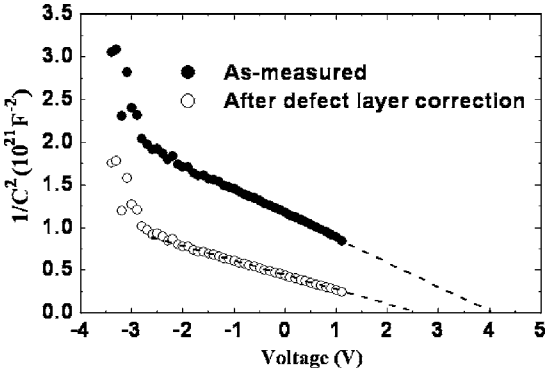

FIG. 3. As-measured and after defect layer correction dependences of C^{-2} vs V of Au/Pt/W_2B/p-GaN Schottky diodes.

culated using the TE model (1.2 eV). In addition, ϕ_B obtained assuming that TFE is similar to that determined from C-V measurements (4.1 eV, see Fig. 3), thus further supporting tunneling-mediated current transport. However, these SBH values are greater than the GaN band gap and are inconsistent with both our XPS measurements and the predictions of the Schottky-Mott model. This discrepancy may be attributed to the presence of an interfacial defect layer. Indeed, it was shown by Shiojima *et al.*[22] using high temperature isothermal capacitance transient spectroscopy that the defects induced by the high Mg doping in p-GaN are essentially located at the surface vicinity and that this region acts as a series capacitance. Therefore, the carriers have to tunnel through an additional barrier, thus resulting in an effective SBH given by $\phi_B = \phi_B^0 + \Delta\phi_B$, where ϕ_B^0 is the true SBH between the contact metal and p-GaN and where $\Delta\phi_B$ is the increment of the SBH due to the presence of the thin defect layer. We have calculated a corrected junction capacitance C_{corr} for W_2B/p-GaN from the equivalent circuit using the simple relation $(1/C_{\mathrm{corr}}) = (1/C_m) - (1/C_d)$, where C_m and C_d are the as-measured and defect layer capacitances, respectively.[22] From our XPS measurements, the true SBH for W_2B/p-GaN is $\phi_B^0 \sim 2.7$ eV. Using our C-V measurements, Fig. 3 shows that the value of C_d required to obtain a SBH similar to that determined by XPS is $C_d \sim 0.70$ nF. Assuming a contact area of $\sim 2 \times 10^{-9}$ m^2 and a relative permittivity of ~ 10, we estimate a defect layer thickness of ~ 0.25 nm, i.e., about 1 ML. For 20 μm diameter diodes, the value of C_d required to fit the XPS data was four times lower than that for 40 μm diameter diodes, as expected from the surface area ratio. The density of acceptors obtained from the corrected C-V's is 1.8×10^{20} cm^{-3}, which is very similar to the value determined from the I-V characteristics.

In summary, we have analyzed the SBH of boride-based rectifying contacts to p-GaN using I-V, C-V, and XPS measurements. I-V's as a function of measurement temperature and comparison of the SBH and the density of acceptors determined from C-V's vs I-V's have demonstrated defect-assisted tunneling as the most dominant mechanism of forward current flow. Consequently, the forward-bias current in boride-based rectifying diodes with high density of acceptors cannot be analyzed using the TE model. However, the SBH determined from TFE is higher than the true SBH for W_2B/p-GaN due to the presence of an interfacial layer acting as an additional barrier to carrier transport.

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