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Citation: J. Appl. Phys. 110, 013716 (2011); doi: 10.1063/1.3607245
View online: http://dx.doi.org/10.1063/1.3607245
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Analysis of leakage current mechanisms in Pt/Au Schottky contact on Ga-polarity GaN by Frenkel-Poole emission and deep level studies

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(Received 22 January 2011; accepted 30 May 2011; published online 12 July 2011)

We report the Frenkel-Poole emission in Pt/Au Schottky contact on Ga-polarity GaN grown by molecular beam epitaxy using current-voltage-temperature (I-V-T) characteristics in the temperature ranging from 200 K to 375 K. Using thermionic emission model, the estimated Schottky barrier height is 0.49 eV at 200 K and 0.83 eV at 375 K, respectively, and it is observed that the barrier height increases with increase in temperature. The extracted emission barrier height (φe) for Ga-polarity GaN Schottky diode by Frenkel-Poole theory is about 0.15 eV. Deep level transient spectroscopy study shows a deep level with activation energy of 0.44 eV, having capture cross-section $6.09 \times 10^{-14}$ cm$^2$, which is located between the metal and semiconductor interface, and trap nature is most probably associated with dislocations in Ga-polarity GaN. The analysis of I-V-T characteristics represents that the leakage current is due to effects of electrical field and temperature on the emission of electron from a trap state near the metal-semiconductor interface into continuum states associated with conductive dislocations in Ga-polarity GaN Schottky diode.

I. INTRODUCTION

Gallium nitride (GaN) is a promising semiconductor material for optoelectronic, high-power, and high-temperature device applications due to its remarkable properties, like wide bandgap, large critical electrical field, and high saturation velocity compared to other semiconductor materials. Device applications include light emitting diodes (LEDs),
laser diodes (LDs),
photo-diodes,
hetero-structure field-effect transistors (HFETs),
and metal-semiconductor field-effect transistors (MSFETs). However, excessive reverse-bias leakage current in Schottky contacts to nitride semiconductor material grown by molecular beam epitaxy remains an outstanding challenge in the development of electronic devices. Several studies on GaN and Al$_x$Ga$_{1-x}$N hetero-structures have shown that the resulting high leakage current in reverse-bias is commonly believed to be tunneling current due to high-density defects and dislocations, which are the primary tunneling paths in GaN film grown hetero-epitaxially on foreign substrates. Some of the researchers reported that the leakage current is dominated by Frenkel-Poole emission (FPE) at a temperature higher than 250 K and carrier transport via conductive dislocations is the dominant source of reverse bias leakage current in GaN hetero-structures. Zhang et al. studied leakage current mechanisms in Schottky contacts on both n-type GaN and AlGa$_x$Ga$_{1-x}$N hetero-structure at different temperatures, and he concluded that tunneling current dominates at low temperatures, whereas FPE dominates at temperatures higher than 250 K.

II. EXPERIMENTAL DETAILS

The Ga-polarity GaN samples for this study were grown by MBE on Si (111) substrate. The epitaxial layers consist of Ga-polarity GaN (1 μm) followed by AlN as intermediate layer (buffer) on Si(111) substrate. The Ohmic metals for GaN, like Ti/Au (20 nm/100 nm), were deposited on a portion of the sample using electron beam evaporation system under a pressure of $4 \times 10^{-6}$ mbar. Then, the Schottky contact was formed by deposition of Pt/Au (20 nm/100 nm) with 1 mm diameter through a mask of circular dots.

Arslan et al. analyzed reverse-bias leakage current mechanisms in Ni/Au Schottky contacts on Al$_{0.83}$In$_{0.17}$N/AlN/GaN hetero-structures in the temperature range of 250 ~ 375 K and reported that the leakage current is due to the emission of electrons from a trapped state near the metal-semiconductor interface into a continuum of states with each conductive dislocation. Recently, Chikhauoi et al. results showed a interface trap with activation energy 0.37 eV, the trap most probably associated with dislocation in AlInN barrier layer. In this work, we studied reverse bias leakage current mechanisms in Pt/Au Schottky contacts on Ga-polarity GaN followed by AlN as intermediate layer (buffer) on Si(111) substrate grown by MBE, using I-V-T characteristics by and FPE model at a temperature ranging from 200 K to 375 K. And also we investigated the deep level defects using deep level transient spectroscopy (DLTS) technique.
Keithley measure unit (Model No. 236) in steps of 25 K from 200 K to 375 K; liquid nitrogen (LN2) cooled cryostat is used for temperature dependent measurement. Capacitance-voltage (C-V) characteristics were measured at room temperature using Boonton capacitance meter (Model No. 7200) and then DLTS measurements were carried out in temperature ranging from 100 K to 400 K using conventional DLTS system having test signal 1 MHz.

III. RESULTS AND DISCUSSION

Figure 2 shows the semi-logarithmic current density as a function of reverse bias voltage for Pt/Au Schottky contact on Ga-polarity GaN in a temperature range of 200°C to 375 K. It is found that reserve leakage current density at 
\[ J = J_s \exp \left( \frac{qV}{nkT} \right) - 1 \]  
(1)

where \( J_s \) is the saturation current density

Here, \( q \) is electron charge, \( V \) is applied voltage, \( n \) is the ideality factor, \( T \) is the absolute temperature, \( k \) is Boltzmann constant, \( A \) is diode area, \( \phi_B \) is the Schottky barrier height (SBH), and \( A^* \) is the effective Richardson’s constant, and it is assumed to be \( 26.4 \text{A cm}^{-2} \text{K}^{-2} \) for GaN.13 The reverse I-V measurement was made to determine saturation current density \( J_s \), from which the barrier height was defined as

\[ \phi_B = \frac{kT}{q} \ln \left( \frac{A^*T^2}{J_s} \right) \]  
(3)

The logarithmic plot of \( J/[1 – \exp(-qV/kT)] \) against \( V \) is linear and \( J_s \) is obtained from the y-axis intercept at zero voltage at each temperature (figure is not shown here). By substituting these \( J_s \) values in Eq. (3), the SBHs were obtained. The extracted SBHs are 0.49 eV at 200 K and 0.83 eV at 375 K, respectively. The inset of Fig.2 shows the plot of barrier height as a function of temperature. The calculated SBH value for each temperature is shown in the table in the inset figure of Fig. 2. It was observed that the SBH increases with increasing temperature, which is commonly observed in real Schottky diodes and has attributed to the barrier in-homogeneity of metal-semiconductor contact.14 Taking into account current transport across the metal-semiconductor interface, electrons at low temperatures can surmount lower SBH, and the dominant current flow is through the regions of lower SBH. When the temperature increases, more and more electrons have sufficient energy to surmount the higher SBH.15,16 Hence, the dominant barrier height increases with temperature.

The Richardson constant \( A^* \) is usually determined from the \( \ln(J_s/T^2) \) versus \( 1000/T \), where \( J_s \) is the saturation current density. Figure 3 shows the conventional Richardson plot. The Richardson constant and effective barrier height at 0 K are obtained from intercept and slope of linear fit. The
effective Richardson constant $A^*$ extracted is 19.98 Acm$^{-2}$K$^{-2}$ and the effective barrier height at 0 K $\phi_B$ (0 K) is 0.10 eV, respectively. Our results are in good agreement to the theoretical effective Richardson constant of GaN (26.4 Acm$^{-2}$K$^{-2}$) and interpreted with Huang et al. reported values of n-GaN. These results may be due to the spatial fluctuations of barrier heights in our contacts. Gue et al. suggested that the decrease in effective contact area may also cause the low value of $A^*$. According to Hacke et al., the Richardson constant is much smaller than the theoretical value, maybe due to presence of a barrier through which the electron is tunnelled. The origin of the high leakage current may lie in different mechanisms, like tunneling, FPE, and generation-recombination. For the temperatures above 250 K, the SBHs are a higher value than 0.57 eV measured from the direct I-V-T characteristics, and we found that the thermionic emission and tunneling over the Schottky barrier in the leakage current is negligible. Hsu et al. and Northrup et al. have shown that conduction related to threading screw dislocations in GaN are the dominant source of high leakage currents at room temperature. In this study, we assume that the main mechanism for leakage current occurs through FPE, and we will focus on reverse bias current density and electric field characteristics.

Leakage current is governed by an emission of electrons via trap state into a continuum of states associated with the presence of conductive dislocations and is successfully explained by the FPE model, in which, usually, the conduction band need not necessarily be in an insulator and its emission refers to the electrical-field-enhanced thermal emission from a trap state into a continuum of electronic states. The current density associated with FPE is given by

$$J = KE_r \exp \left[ -\frac{q \left( \phi_r - \sqrt{\frac{qE_r}{kT}} \right)}{kT} \right], \quad (4)$$

where $E_r$ is the electric field in the semiconductor barrier at the metal/semiconductor interface, $\phi_r$ is the barrier height for electron emission from the trapped state, $\varepsilon_0$ is the relative dielectric permittivity, $T$ is the absolute temperature, $\varepsilon_{\mathrm{so}}$ is the permittivity of free space, $k$ is the Boltzmann’s constant, and $K$ is a constant. From Eq. (4), $\ln(J/E_r)$ should be a linear function of $\sqrt{E_r}$, i.e.,

$$\ln(J/E_r) = \frac{q}{kT} \sqrt{\frac{qE_r}{\pi \varepsilon_0 \varepsilon_r}} - \frac{q \phi_r}{kT} + \ln C = A(T) \sqrt{E_r} + B(T),$$

(5a)

where

$$A(T) = \frac{q}{kT} \sqrt{\frac{q}{\pi \varepsilon_0 \varepsilon_r}}, \quad (5b)$$

$$B(T) = -\frac{q \phi_r}{kT} + \ln C. \quad (5c)$$

Figure 4 shows the plot of $\ln(J/E_r)$ versus $\sqrt{E_r}$ as linear in the temperature range 200 $\sim$ 375 K for Pt/Au Schottky contact on Ga-polarity GaN; this is a proof for a Frenkel-Poole effect in Pt/Au Schottky contacts on Ga-polarity GaN. As defined in Eqs. (5b) and (5c), we also plotted $A(T)$ and $B(T)$ as functions of $1/T$ for the Au/Pt/GaN Schottky diode. The calculated relative dielectric constant from the slope of $A(T)$ versus $1000/T$ (figure is not shown here) is 3.2 and the emission barrier $\phi_r$ from the slope of $B(T)$ versus $1000/T$ (the inset of Fig. 4) is 0.15 eV, respectively. The extracted value of $\phi_r$ for Ga-polarity GaN is in good agreement with the previously reported values rather than the 9.5. Poole effect in Pt/Au Schottky contacts on Ga-polarity GaN; this is a proof for a Frenkel-Poole effect in Pt/Au Schottky contacts on Ga-polarity GaN. As defined in Eqs. (5b) and (5c), we also plotted $A(T)$ and $B(T)$ as functions of $1/T$ for the Au/Pt/GaN Schottky diode. The calculated relative dielectric constant from the slope of $A(T)$ versus $1000/T$ (figure is not shown here) is 3.2 and the emission barrier $\phi_r$ from the slope of $B(T)$ versus $1000/T$ (the inset of Fig. 4) is 0.15 eV, respectively. The extracted value of $\phi_r$ for Ga-polarity GaN is in good agreement with the previously reported values rather than the 9.5. Recently, Arslan et al. reported that dielectric constant and emission barrier are 5.8 and 0.12 eV for AlInN/AlN/GaN hetero-structures, respectively. Further supporting the validity of FPE, DLTS measurement was performed.

DLTS is one of the most sensitive tools for detection and characterization of electrically active defects in a semiconductor thin film Schottky-junction and p-n junction device structure. DLTS measurements were carried out in a temperature range of 100 $\sim$ 300 K. Prior to the DLTS measurements, the diode was first examined by C-V measurement. The estimated carrier concentration from slope of $1/C^2$ versus $V$ was $\sim 4.92 \times 10^{19}$/cm$^2$. For DLTS measurement, the sample was biased at $-4$ V ($V_r$) and periodically pulsed at $-1$ V ($V_{pp}$) for trap filling. The transient capacitance signal, acquired by using a test ac signal of 1 MHz with an emission rate window of 0.065 s$^{-1}$ were recorded in a temperature range of 100 $\sim$ 300 K and the measured spectrum, as shown in Fig. 5; there were no peaks observed above 200 K in DLTS spectrum. The activation energy and capture cross section of deep level defect were obtained from the Arrhenius plot, which was plotted from DLTS signals at different rate windows. According to the principle of detailed balance, the electron emission time $\tau_n$ related with trap parameters is given by

$$\tau_n^{-1} = \sigma_n \gamma_e T^2 \exp \left(-\frac{E_T}{kT} \right), \quad (6)$$

where $\sigma_n$ is the capture cross section, $\gamma_e$ is a constant, $k$ is the Boltzmann constant, and $E_T$ is the trap activation energy.
current density, which are determined through the emission into or from dislocation-related trap states, in which carrier transport from the metal contact into the conductive dislocation must occur via a trapped state rather than a thermionic emission from the metal.

IV. CONCLUSIONS

We have discussed leakage current mechanisms across the Pt/Au Schottky contact on Ga-polarity GaN grown by MBE on Si(111) substrate using I-V measurements in the temperature ranging from 200 K to 375 K by thermionic emission and FPE models. The calculated SBH is 0.49 eV at 200 K and 0.83 eV at 375 K, respectively. The estimated electron emission barrier height is about 0.15 eV. DLTS measurement showed a dominating defect level with activation energy 0.44 eV having capture cross-section $6.09 \times 10^{-14} \text{cm}^2$ below the conduction band, the defect most probably associated with dislocations in Ga-polarity GaN. The analysis of reverse I-V characteristics indicates that the leakage current flow above 250 K is due to the emission of electrons from a trapped state near the metal-semiconductor interface into or from a continuum of states which are associated with conductive dislocation.

ACKNOWLEDGMENTS

This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF), funded by the Ministry of Education, Science and Technology (2010-0023852), and by the National Research Foundation of Korea Grant funded by the Korean Government (MEST) (NRF-M1AWA001-2010-0026292).