Temperature dependent electrical studies on Cu/AlGaN/GaN Schottky barrier diodes with its microstructural characterization

Manjari Garg [a], Ashutosh Kumar [a, *, 1], Haiding Sun [b, 2], Che-Hao Liao [b], Xiaohang Li [b], Rajendra Singh [a, c, **]

[a] Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India
[b] Advanced Semiconductor Laboratory, King Abdullah University of Science and Technology (KAUST), Thuwal, 23955-6900, Saudi Arabia
[c] Nanoscale Research Facility, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India

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ABSTRACT

The performance of the AlGaN/GaN heterostructure based devices depends largely upon electrical behavior of Schottky contact which controls the current flowing through the channel. In this work, electrical behavior of Copper (Cu) Schottky diodes on $Al_{0.25}Ga_{0.75}N$/GaN heterostructures grown on Silicon have been investigated using temperature dependent current-voltage (I-V) and capacitance-voltage (C-V) techniques. An ideality factor (η) of 1.3 at room temperature (RT) signified that the forward current is dominated by thermionic emission process for current flow in the Schottky diode. The strong polarization field effects with in the barrier layer of the strained AlGaN/GaN heterostructure were considered for evaluating the barrier height using C-V measurements. The barrier height from such analysis was found to be 1.66 eV at RT which is significantly higher than theoretically predicted barrier height for Cu/AlGaN/GaN Schottky diodes. This observation of high barrier height is attributed to the presence of an ultra-thin Cu_2O layer between Cu and AlGaN layer as revealed from scanning transmission electron microscopy. The temperature dependence of the barrier height suggests inhomogeneous nature of the Cu/AlGaN/GaN interface with different level of barrier inhomogeneities in different temperature ranges. Further, frequency-dependent C-V measurements were used to electrically characterize surface traps at Cu/AlGaN/GaN interface. Present study highlights the potential of Cu as a Schottky contact on AlGaN/GaN heterostructures for achieving high barrier height which is of utmost importance in GaN based device technology.

1. Introduction

Group III-Nitride based AlGaN/GaN high electron mobility transistors (HEMTs) are one of the most promising candidates for high-power and high-frequency microelectronic device fabrication owing to their superior material properties [1–5]. They possess a large band gap, high breakdown fields, high peak and saturation electron drift velocities, and high sheet charge densities on the order of 10^{13} cm^{-2} at the interface [6–8]. In HEMTs for power applications, Schottky (gate) electrode with a higher barrier height is suitable to achieve maximum drain current, high transconductance, high turn-on voltages and high breakdown voltage of the device. It also results in small gate leakage current, thus reducing the noise level. In existing reports, Schottky barrier contacts on AlGaN/GaN HEMTs using high work function metals like Platinum [9] Iridium [10,11], Nickel [11–14], Palladium [15] etc. capped by gold metallization have been reported. Copper (work function (ϕ_m) ~ 4.65 eV) was introduced as a Schottky metal contact on n-Si and p-Si by Aboelfotoh et al. in 1990 [16]. The variable temperature current-voltage (I-V) measurements and calculations based on thermionic emission theory of current transport were performed on these diodes. The room temperature ideality factor of 1.01 and barrier height of 0.6 eV, evaluated by considering thermionic emission as the dominant current transport mechanism

suggested that fabricated Cu/n-Si and Cu/p-Si Schottky diodes were of good quality. Later Ao et al. [17] extended the use of Cu as a gate material to n-GaN and AlGaN/GaN epitaxial films, and found lower gate leakage current in comparison to devices with Ni/Au as the gate material [17,18]. This improvement in the leakage current was attributed to lesser Cu diffusion as observed from conducting secondary ion mass spectrometry. In addition, Cu-gated AlGaN/GaN HEMTs were found to the thermally stable as devices were found to be stable when annealed at 500 °C for 1 h. Following this, Esposto et al. [19] studied the influence of interface states at the Schottky junction on the large signal behavior of the Cu-gated HEMTs. Through numerical simulations and analysis of drain current transients, they revealed the presence of an acceptor trap with activation energy of 0.43 eV in the AlGaN barrier beneath the Cu/AlGaN Schottky junction. All of the above-mentioned reports suggest the potential of Cu as a Schottky contact on AlGaN/GaN heterostructures, however current transport in these reports is limited to room temperature. The room temperature I-V characteristics does not give detailed information about the nature of the barrier formed or the current transport process at the MS interface. The temperature dependence of the I-V characteristics helps to understand different aspects of the conduction mechanisms like departure from the pure thermionic emission, homogenous or inhomogeneous nature of the barrier with quantitative estimation of level of barrier inhomogeneities at the MS interface. For understanding electron transport at Cu/AlGaN/GaN interface, temperature dependent I-V measurements have been carried out in the present study. In addition to this, strained AlGaN/GaN heterostructures have strong polarization field with in the AlGaN barrier due to which the barrier height calculation from conventional thermionic emission theory may not be appropriate. Hence, in this work, an approach which considers the polarization effects has been used for estimating barrier height of Cu/AlGaN/GaN Schottky barrier diodes.

2. Experimental

The $Al_{0.25}Ga_{0.75}N$/GaN HEMT structure used in this study was grown by metal organic chemical vapor deposition (MOCVD) technique. The HEMT structure was grown on silicon (111) substrate. All layers were grown with unintentional doping. The HEMT structure began with 100 nm thick AlN nucleation layer deposited on the substrate. Next, a 1 μm thick graded (95%–0%) $Al_{1-x}Ga_xN$ buffer layer was deposited. Then a 2 μm thick high mobility GaN channel layer was deposited followed by deposition of a 1 nm AlN spacer layer and a 25 nm undoped $Al_{0.25}Ga_{0.75}N$ donor layer. The structure was then capped by a 2 nm GaN cap layer. The two-dimensional electron gas (2DEG) formed at the AlGaN/GaN interface was characterized electrically with electron mobility of about 1800 cm^2/V, sheet carrier concentration of about 1.14×10^{13} cm^{-2} and sheet resistance of about 384 Ω/square at room temperature. The sample pieces were cleaned using De-ionized (DI) water, acetone and boiling Iso-Propanol for 5 min each in an ultrasonic bath cleaner. The samples were then rinsed by DI-water. The native oxide layer on the surface was etched by dipping the samples in a solution of hydrochloric acid and DI-Water (ratio 1:2) for 30 s. The etched samples were cleaned using DI-Water for a long time and dried using nitrogen jet. After this procedure, the samples were loaded into the evaporation deposition chamber, immediately. For ohmic contact, Ti/Al/Ni/Au (300/1500/400/1000 Å) metal stack was evaporated using e-beam evaporation at a base pressure of 10^{-8} Torr on the four corners of the samples and thermally annealed at 800 °C for 60 s in N_2 ambiance. In the next step, Cu(40 nm)/Au(100 nm) metals were deposited on the polished side of the samples as circular dots with diameter of 2 mm as Schottky

contacts using a thermal evaporation system at the base pressure of 10^{-6} Torr. The deposition rate was about 1 $Ås^{-1}$. The I-V characteristics were measured using a home-made LN_2 cryostat and Keithley Semiconductor Characterization System (SCS-4200). The measurements were performed at different temperatures in the temperature range of 80–340 K (step size ~ 20 K). During each measurement, the temperature was controlled and stabilized within ±1 K, using Cryocon Temperature controller (Model 32). The scanning transmission electron microscopy (STEM) was utilized to investigate the interface by operating a probe corrected FEI Titan system at an acceleration voltage of 300 kV. The STEM specimens were prepared by an FEI Helios G4 dual beam focused ion beam (FIB) equipped with an omniprobe.

3. Results and discussion

The *logI-V* characteristics of Cu/AlGaN/GaN Schottky barrier diodes as a function of temperature have been plotted in Fig. 1. The rectification ratio at ±5 V is ~10^6 in the temperature range of 280–340 K, however it tends to decrease with the decrease in temperature. At lower forward bias, a small increase in gate current is observed with increase in temperature, but the plots tend to merge at higher forward bias. For thermionic emission (TE) current transport at V > 3kT/q the current flowing across the MS interface is given by Ref. [20].

$$I = \left[AA^*T^2 exp\left(-\frac{q\phi_B}{kT} \right) \right] \left[exp\left(\frac{qV}{\eta kT} \right) - 1 \right] \tag{1}$$

where A is the area of the Schottky diode, A^* is the effective Richardson coefficient, T is the absolute temperature, q is the fundamental electronic charge, ϕ_B is the barrier height, k is the Boltzmann's constant, V is the applied voltage and η is the ideality factor. The value of η, extracted from the slope of $log(I)$ versus V plot (for V > 3kT/q) was found to be 1.3 at room temperature. However, barrier height calculation from conventional thermionic emission current transport may not be appropriate due to presence of strong polarization field within the strained AlGaN barrier. The polarization field in the strained AlGaN layer induces charges at the AlGaN/GaN interface. The electrons of the AlGaN surface states flow to the AlGaN/GaN interface forming the two-dimensional electron gas (2DEG) at the heterojunction [21]. Thus the barrier height of the
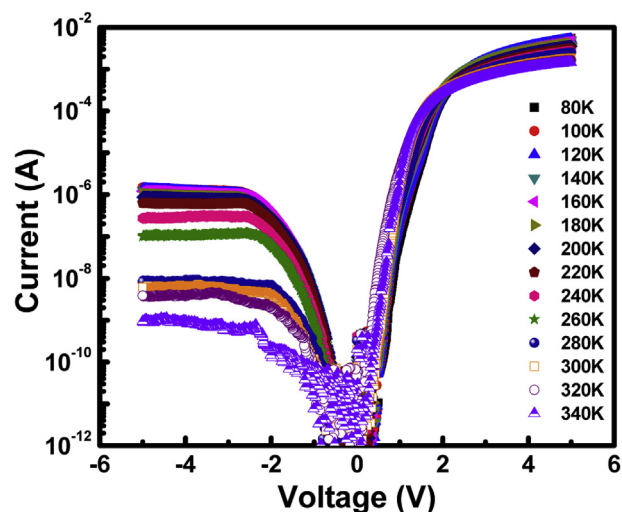

Fig. 1. Measured current-voltage (I-V) characteristics of Cu/AlGaN/GaN Schottky barrier diode in the temperature range of 80–340 K.

Schottky diode is strongly related to the sheet charge density of the 2DEG. For an undoped HEMT heterostructure with a Schottky gate contact, the 2DEG sheet carrier concentration at the AlGaN/GaN interface is given by Ref. [22].

$$n_s(x) = \frac{\sigma(x)}{q} - \left[\frac{\varepsilon_o \varepsilon_s(x)}{dq^2}\right][e\phi_b(x) + E_F(x) - \triangle E_c(x)] \tag{2}$$

where x is the Al concentration, σ is the polarization sheet charge density, q is electron charge, ε_o is the permittivity of free space, ε_s is the relative dielectric constant of AlGaN barrier layer, d is the width of AlGaN, $e\phi_b$ is the Schottky barrier height, E_F is the Fermi level with respect to the GaN conduction-band-edge energy, and $\triangle E_c$ is the conduction band offset at the AlGaN/GaN interface. The Fermi level $E_F(x)$ is given by Ref. [23].

$$E_F(x) = \left[\frac{\pi\hbar^2 n_s(x)}{m^*(x)}\right] + \left[\frac{9\pi\hbar e^2}{8\varepsilon_o\sqrt{8m^*(x)}}\frac{n_s(x)}{\varepsilon(x)}\right]^{2/3} \tag{3}$$

where $m^*(x)$ is the effective mass of the electron. The band offset $\Delta E_c(x)$ for AlGaN/GaN heterointerface is determined by Refs. [24–26].

$$\triangle E_c = 0.7[6.31x + 3.42(1-x) - x(1-x) - E_g(0)] \tag{4}$$

If x is taken as 0.25 (as in our work), the band offset $\triangle E_c(x)$ is calculated to be 0.343 eV. The sheet carrier concentration $n_s(x)$ was calculated from capacitance-voltage (C–V) profiling. Fig. 2 shows the measured C-V characteristics of Cu Schottky contacts on strained $Al_{0.25}Ga_{0.75}N$/GaN heterostructure at a frequency of 1 MHz at different temperatures. It can be seen from the figure that the channel is pinched-off below -2 V and fully open at 0 V. From the data of C-V measurement, the apparent carrier concentration versus depletion depth (N_{CV}-ω) profile was deduced using the relation: $N_{CV} = C^3/\{q\varepsilon A^2(dC/dV)\}$ and $\omega = A\varepsilon_o\varepsilon_s$/Then $n_s(x)$ was calculated by integrating the apparent carrier concentration with respect to depletion depth ($n_s = \int_{-\infty}^{\infty} N_{CV}(\omega)d\omega$). [27,28] The calculated 2DEG sheet carrier concentration at the AlGaN/GaN interface was calculated as 6.3×10^{12} cm^{-2} at room temperature. Using effective mass, $m^*(x) \approx 0.22m_e$, $\varepsilon(x)$ as 10.33, $\sigma(x)$ as 9.8×10^{12} cm^{-2} [29] and the AlGaN layer thickness $d = 25$ nm, Schottky barrier height of 1.66 eV was calculated at room temperature. The E-x
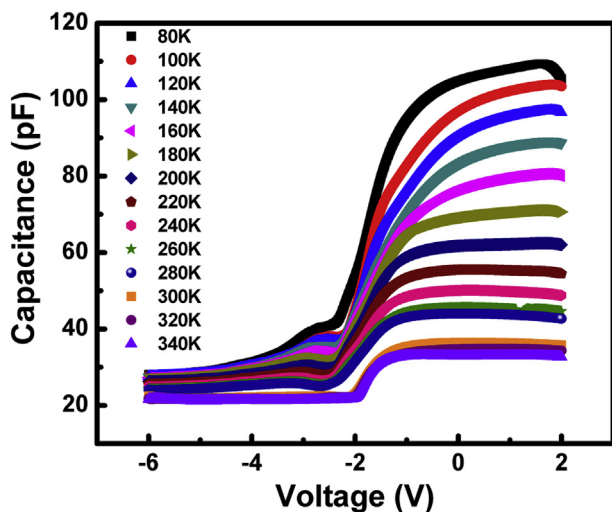

Fig. 2. Measured capacitance-voltage (C-V) curves of Cu/AlGaN/GaN Schottky barrier diode at 1 MHz in the temperature range of 80–340 K.

diagrams of the Cu/AlGaN/GaN MS interface after the junction formation and under forward bias are proposed in Fig. 3.

Next, we compared the observed barrier height for Cu/AlGaN/GaN Schottky contacts with the barrier height predicted as per Schottky-Mott model [20]. As per this model, barrier height for Cu/AlGAN/GaN Schottky contacts is given as ∼ $\sim \phi_{Cu} - \chi_{AlGaN}$ where ϕ_{Cu} is the work function of the Cu and χ_{AlGaN} is the electron affinity of the AlGaN layer. In this work, χ_{AlGaN} is estimated by assuming a linear dependence of electron affinity of $Al_xGa_{1-x}N$ on the Al fraction, x. By choosing $\chi_{GaN} = 4.20$ eV and $\chi_{AlN} = 2.05$ eV [30,31], χ_{AlGaN} comes out to be 3.67 eV for x = 0.25. For ϕ_{Cu} of 4.65 eV and χ_{AlGaN} (x = 0.25) ∼3.67 eV, Schottky-Mott model predicts barrier height to be close to 1.0 eV. The other factors like existence of interface states and barrier inhomogeneities tends to further lower this barrier height [32,33], hence observed barrier height for Cu/AlGaN/GaN Schottky contacts should be lower than 1.0 eV. However, observed room temperature barrier height of 1.66 eV for this system is significantly higher than this expected barrier height. To explain this discrepancy, we have carried out STEM-based microstructural investigation of Cu/AlGaN/GaN interface. The Schematic of the Au/Cu/AlGaN/GaN sample is shown in Fig. 4(a) where investigated region is marked with a box. Fig. 4(b) shows the cross-sectional view of the Cu/AlGaN/GaN interface with (c) representing the magnified view. In (c), a Cu_2O oxide layer of about 3 nm is seen between the Cu and AlGaN surface. The presence of this oxide layer is likely to affect the electrical transport across the Cu/AlGaN interface. One possibility behind the formation of this oxide layer may be the unintentional chemical reaction between the Cu metal and the native oxide of the GaN. In as-deposited form, Cu_2O behaves as the p-type semiconductor with band gap ∼2.1 eV and χ of 2.9 eV [34]. With a high work function of about 5.36 eV as experimentally observed by Soon et al. [35], Cu_2O behaves as the degenerate semiconductor. The formation of Cu_2O layer transforms Cu/AlGaN system to Cu/p + -Cu_2O/AlGaN systems. The barrier height of such system is expected to be ∼1.70 eV which is in close agreement with our observed barrier height of 1.66 eV.

To further understand the electronic transport and investigating the impact of barrier inhomogeneities, I-V measurements are carried out in the temperature range of 80–340 K. values of ideality factor (η) and apparent Schottky barrier height (ϕ_{Bo}) were evaluated at each temperature using Eq. (1) in a similar manner as described earlier in this manuscript. Fig. 5 shows the variation of ϕ_{Bo} and η with temperature where η decreases while ϕ_{bo} increases with increase in temperature. This behavior is attributed to the existence of Schottky barrier inhomogeneities at MS interface [36–41]. One major reason behind the origin of Schottky barrier inhomogeneities is that the metal contacts are not epitaxially grown on AlGaN/GaN surface. Due to this, interface is not atomically flat but rough which causes electric field to vary locally, giving rise to barrier inhomogeneity. The other reason for these inhomogeneities are believed to be surface traps, vacancy-related defects, threading dislocations, metal-induced gap states, interface states, etc. [40–44] Due to these inhomogeneities, Schottky barrier height follows a distribution which is directly linked with the potential fluctuations at the MS interfaces, as demonstrated experimentally using nanoscopic electrical characterizations in our recent work on similar sample [9]. As a consequence of these inhomogeneities, electronic transport at lower temperatures is dominated by electrons crossing the barriers having lower barrier height. As temperature increases, electrons tend to cross the barriers with higher barrier height as they have sufficient energy. The electronic transport under the existence of barrier inhomogeneities at MS interface was explained by J. H. Werner and H. H. Guttler in the form of Gaussian distribution of ϕ_{bo} with standard deviation σ_s around mean barrier height $\overline{\phi_{bo}}$ as [45].
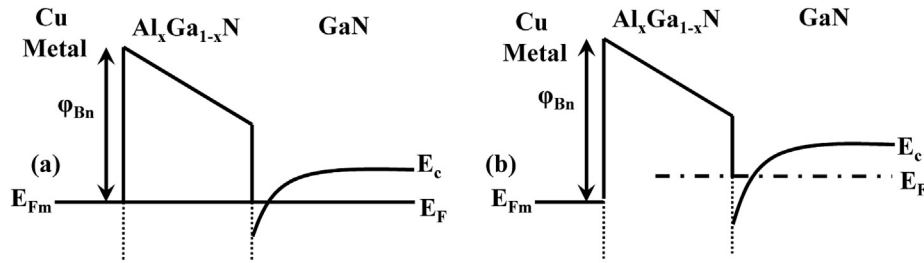
Fig. 3. Proposed E-x diagram showing the Cu/AlGaN/GaN metal semiconductor interface (a) at zero bias (b) under forward bias.
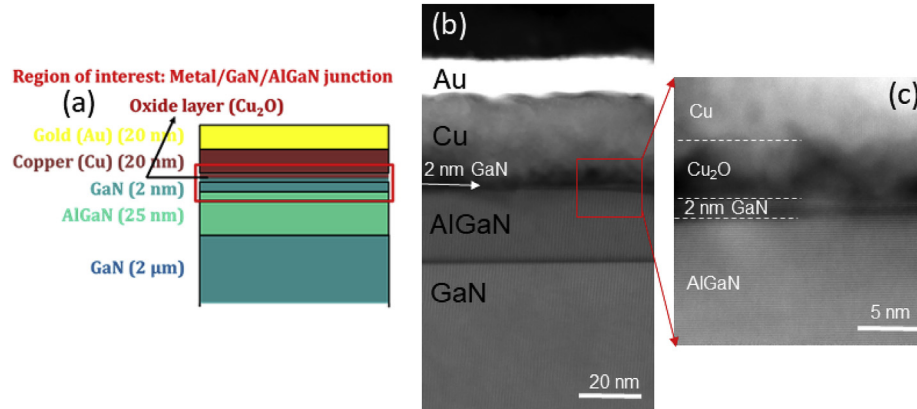

Fig. 4. (a) Schematic of the sample investigated showing the region of interest. Scanning transmission electron microscopic image of Cu/AlGaN/GaN interface is shown in (b) with (c) showing the magnified view, where a Cu_2O layer of about 3 nm is clearly seen.
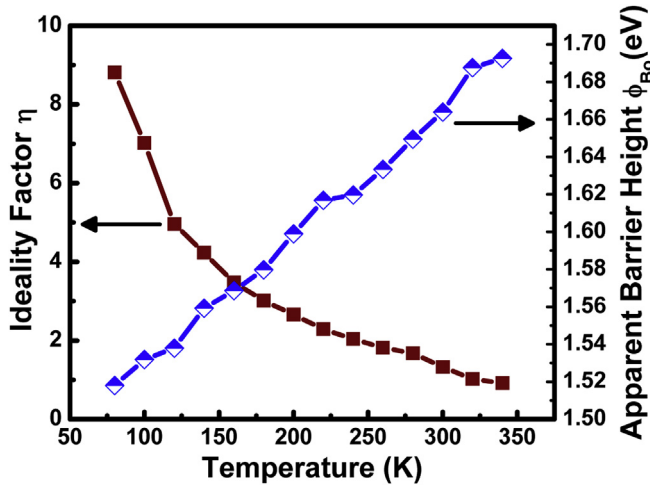

Fig. 5. Variation of ideality factor and barrier height with temperature in the range of 80—340 K. The increase in ideality factor with decrease in temperature indicates the departure from pure thermionic emission transport at lower temperatures while lower of barrier height with lowering in temperature is primarily attributed to the inhomogeneous nature of Cu/AlGaN/GaN MS interface.

Fig. 6. Variation of ϕ_{Bo} with $(2\,kT)^{-1}$ showing the existence of two linear regions in the temperature ranges 80—160 K and 160—340 K. The circular points represent the experimental data while solid lines represent the linear fitting, considering the Gaussian distribution of local barrier heights.

$$\phi_{bo} = \overline{\phi_{bo}} - \frac{\sigma_s^2}{2kT} \tag{5}$$

According to Eq. (5), the values of σ_s and $\overline{\phi_{bo}}$ can be calculated from the slope and y-intercept of the plot between ϕ_{bo} (in eV) and $2\,kT^{-1}$ (in eV^{-1}). Fig. 6 shows the ϕ_{bo} versus $(2\,kT)^{-1}$ plot in the temperature range of 80—340 K, where two straight line regions (80—160 K and 16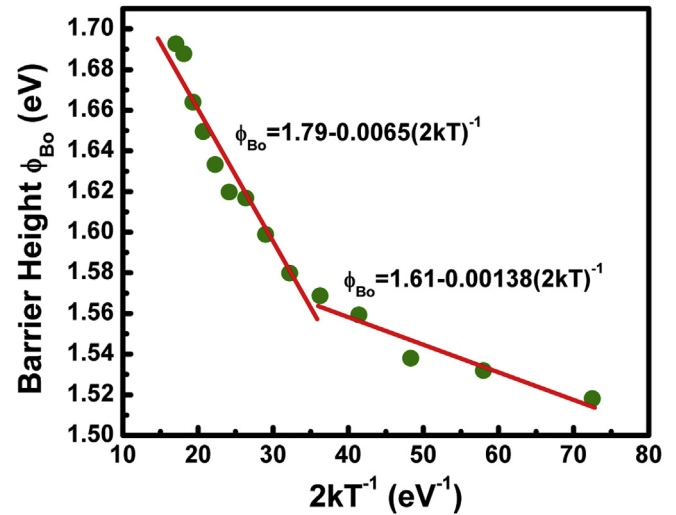0—340 K) with different slopes and intercepts are observed. From slopes and y-intercepts of these straight lines, $\overline{\phi_{bo}}$ and σ_s were calculated as 1.79 eV and 80.6 meV in the temperature range of 160—340 K and 1.61 eV and 37.1 meV in the temperature range of 80—160 K, respectively. The width of Gaussian distribution, σ_s gives the level of barrier inhomogeneities at MS interface. As $\sigma_s \sim 80.6$ meV in temperature range of 160—340 K is higher than $\sigma_s \sim 37.1$ meV in temperature range 80—160 K, it suggests more inhomogeneous nature of the interface in higher temperature

range of 160–340 K in comparison to lower temperature range of 80–160 K. It is worth mentioning here that the level of barrier inhomogeneities, σ_s ~80.6 meV estimated here in the temperature range 160–340 K is similar to the value of σ_s ~85 meV estimated using nanoscopic electrical characterizations in our recent work on the similar sample where Pt has been used a Schottky contact [9].

The surface trap states which were one of the reasons for spatial inhomogeneity of the Schottky barrier are even the cause for capacitance dispersion. A change of charge in the trap states occurs when the trap levels crosses the Fermi level resulting in an additional capacitance at a macro level. However, the trap states cannot contribute to the capacitance at high frequency since the associated charge cannot follow the high frequency signal. The measured capacitance only consists of space charge capacitance ($C \cong C_{sc}$). At low frequencies, the contribution of the interface states to diode capacitance decreases with increasing frequency. Experimentally measured capacitance corresponding to low frequency in the C-f measurements data is approximately equal to the sum of the space charge capacitance and the interface capacitance (C_{int}) ($C = C_{sc} + C_{int}$). [46,47,48] In order to understand the trap behavior behind the capacitance dispersion, a simplified model has been proposed by Nicollian and Goetzberger. [49] As per this model, interface-state capacitance (C_{int}) can be described as

$$C_{int} = AqN_{int}\frac{\arctan(\omega\tau)}{\omega\tau} \tag{6}$$

where N_{int} is the effective trap states density, ω is the radian frequency, and τ is the time constant, respectively. Fig. 7 shows the measured capacitance as a function of radian frequency at the bias voltage of -2 V (pinch-off voltage). The experimental curve was numerically fitted with eq. (6) to obtain the effective trap density and time constant. The fitting results are shown as the solid line in Fig. 6. The effective trap density calculated at the pinch-off voltage is approximately 4.21×10^{11} cm^{-2} eV^{-1} and the time constant is 8.7 μs. The estimation of effective trap density and their time constant may help in understanding the spatial inhomogeneity and its impact on electrical transport across Cu/AlGaN/GaN interface.
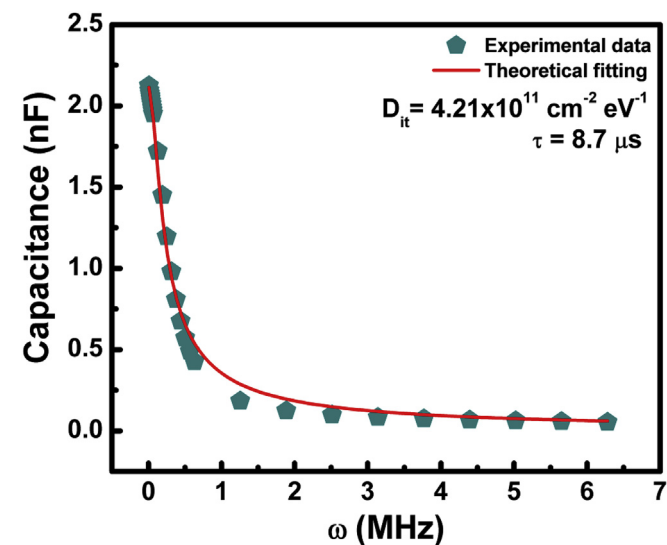

Fig. 7. Frequency sweep C-V measurement data from 1 kHz to 1 MHz (shown by pentagon shaped points) while solid line represents theoretical fitting of the measured data using Eq. (6) at the gate bias of -2 V (pinch-off voltage).

4. Conclusions

Temperature dependent current-voltage and capacitance-voltage measurements have been employed to understand the electrical behavior of Cu/Al$_{0.25}$Ga$_{0.75}$N/GaN Schottky barrier diodes. Using thermionic emission current mechanism in the forward bias, ideality factor (η) of 1.3 at room temperature was calculated, indicating the good quality of the fabricated diodes. A different approach based on capacitance-voltage measurement which considers the polarization effects in the barrier layer has been used to calculate the Schottky barrier height (ϕ_{bo}). From scanning transmission electron microscopy, a Cu$_2$O layer of about 3 nm thickness is observed between Cu and AlGaN/GaN which explains the high barrier height ~1.66 eV, observed for Cu/AlGaN/GaN Schottky barrier diode. The temperature dependence of η and ϕ_{bo} implied spatial inhomogeneity of barrier height at the interface which is estimated by considering Gaussian distribution of ϕ_{bo} with standard deviation σ_s around mean barrier height $\overline{\phi_{bo}}$. The value of mean barrier height and standard deviation were calculated as 1.79 eV and 80.6 meV in the temperature range of 160–340 K and 1.61 eV and 37.1 meV in the temperature range of 80–160 K respectively. In addition, surface trap density of 4.21×10^{11} cm^{-2} eV^{-1} with time constant of 8.7 μs was also evaluated using frequency dependence of C-V data. The quantitative estimation of level of barrier inhomogeneities at Cu/AlGaN/GaN interface, surface trap densities analysis and microstructural investigations in our study may prove beneficial for further understanding of electronic transport in Cu based Schottky contacts on GaN based heterostructures.

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