Effective Schottky Barrier Height Model for N-Polar and Ga-Polar GaN by Polarization-Induced Surface Charges with Finite Thickness

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The nitrogen-polar GaN material system is a promising candidate for high-frequency applications, such as those in the millimeter-wave range. Schottky barrier height is one of fundamental parameters necessary for device applications of N-polar GaN. Herein, vertical Schottky diodes for both N-polar and Ga-polar GaN are prepared, and it is found through experiments that the barrier height of N-polar GaN is smaller than that of Ga-polar GaN by 0.21 V. This difference in the barrier height stems from the polarization-induced surface charge layer of a few angstroms thickness under the surface. Numerical calculation of band profiles suggests that a significant band bending caused by the large amount of polarization charges pushes the conduction band energy downward (upward) in the N-polar (Ga-polar) surface depending on the sign of the polarization charges, which results in two different effective Schottky barrier heights. This difference is explained by assuming the polarization-charge layer thickness of about 5 Å. A simple analytical model to estimate the difference in barrier heights between the two polarities is also proposed.

1. Introduction

GaN-based high-electron mobility transistors (HEMTs) have been extensively studied in power applications with high operation frequencies. In particular, the desire for application to wireless telecommunication system base stations has become a driving force in the development of GaN power devices.[1] For application of GaN HEMTs to next-generation telecommunication systems, we need to explore higher frequency ranges, such as the millimeter-wave and submillimeter-wave ranges. For such purposes, the gate length of HEMTs must be shrunk to achieve higher frequency performance. Moreover, to maintain electrostatic control in such short-gate HEMTs, the gate–channel distance needs to be reduced so that the device dimensions maintain an appropriate aspect ratio. The nitrogen-polar GaN material system is a promising candidate for such high-frequency applications due to the natural back barrier provided by GaN/AlGaN heterostructures. In N-polar GaN HEMTs, due to the opposite sign of the polarization-induced surface charges, 2D electron gas is formed at the interface of GaN and AlGaN in the case where the GaN channel is on top of the AlGaN layer.[2] This helps reduce the gate–channel distance in HEMTs, and the back barrier provided by the AlGaN layer makes the carrier confinement stronger in comparison with Ga-polar GaN HEMTs.

Successful growth[3,4] and device application[5–8] of N-polar GaN materials have been reported from different groups. In particular, the superior power performance of N-polar GaN HEMTs compared with their Ga-polar counterparts has been demonstrated in high frequencies over 90 GHz.[6] To exploit the full potential of N-polar GaN, we need to clarify its material properties, particularly ones that are different from those obtained by Ga-polar materials. One such property is Schottky barrier height.

In this work, we report our experimental characterization of the Schottky barrier height of N-polar and Ga-polar GaN and propose a simple physical model to represent the different Schottky barrier heights between the two polarities. Starting from a common intrinsic Schottky barrier height, the proposed model describes the difference in the effective barrier height between N-polar and Ga-polar GaN by considering the significant band bending caused by the polarization-induced surface charge layer of a few angstroms thickness under the surface.

2. Experimental Section

2.1. Sample Preparation

The quality of N-polar epitaxial film was sufficient to form 2D electron gas by means of a GaN/AlGaN/GaN inverted HEMT structure.[8] In this sample preparation, we grew an unintentionally doped N-polar GaN layer on the carbon face of...
an n-type SiC substrate by metalorganic vapor-phase epitaxy (MOVPE). The thickness of the GaN layer was 1.2 μm. Using this material, vertical Schottky diodes were fabricated to characterize the Schottky barrier height. First, ohmic electrodes were formed on the underside of the sample. After cleaning the sample with diluted hydrochloric acid (HCl:H₂O = 1:1), Ti/Pt/Au metal stacks were evaporated, and annealing was performed at 780 °C for 2 min in nitrogen ambient. Next, Schottky electrodes were formed on the top of the sample by evaporating Ni/Au metal stacks following the sample cleaning with diluted hydrochloric acid. For comparison, we also prepared Schottky diodes using a standard Ga-polar GaN. The Ga-polar GaN epitaxial film consisted of a 2 μm-thick lightly doped GaN layer (estimated Si doping concentration: 6.5 × 10¹⁶ cm⁻³) on a 1 μm-thick heavily doped GaN layer (doping concentration: 2 × 10¹⁸ cm⁻³) grown on an n-type freestanding GaN substrate.

2.2. Evaluation of Schottky Barrier Height

2.2.1. Current–Voltage Characteristics

We measured the on-wafer DC current density versus voltage (J–V) characteristics at room temperature using a Keysight B1505A parametric power device analyzer with a Cascade EPS150 probe station. The Schottky barrier height (φₜₐ₈) was obtained from the J–V characteristics under a sufficiently large forward bias condition (V > 3kT/q) using the following thermionic emission model

\[ J = A^*T^2 \exp\left(\frac{-q\phi_{bi}}{kT}\right) \exp\left(\frac{qV}{nkT}\right) \]  

where q is the elementary charge, k is the Boltzmann constant, T is the temperature, n is the ideality factor, and A* is the effective Richardson constant (240 A cm⁻² K⁻² for GaN)[9]. The measured J–V characteristics were fitted using Equation (1) to obtain the barrier height (φₜₐ₈) and ideality factor (n).

2.2.2. Capacitance–Voltage Characteristics

We also estimated the Schottky barrier height by means of the capacitance versus voltage (C–V) characteristics under the reverse bias condition. The C–V characteristics were measured in the capacitance measurement unit of B1505A at the frequency of 1 MHz. The correlation between the depletion-layer capacitance per unit area C and the applied voltage V is given as[10]

\[ \frac{1}{C} = \frac{2}{\varepsilon_s N_D} \left( \psi_{bi} - V - \frac{kT}{q} \right) \]  

where εₛ is the permittivity in GaN (8.9 × permittivity in vacuum) [11], ψₜₐ₈ is the built-in potential, and N_D is the donor concentration. From Equation (2), the slope and the intercept value of the (1/C²)–V plot give the donor concentration (N_D) and the built-in potential (ψₜₐ₈), respectively. The barrier height (φₜₐ₈) can be obtained from the built-in potential and the Fermi potential from the conduction band edge (φₚₑₐ₈), as shown in Figure 1. That is

\[ \phi_{bi} = \psi_{bi} + \phi_{p}\ ]

\[ \phi_{bi} = \psi_{bi} + \frac{kT}{q} \ln \left( \frac{N_C}{N_D} \right) \]

where N_C is the effective density of states in the conduction band of GaN (2.3 × 10²⁰ cm⁻³ at room temperature)[11].

3. Results and Discussion

3.1. Experimental Values of Schottky Barrier Height

Figure 2 shows the typical forward J–V characteristics of the N-polar and the Ga-polar GaN samples in logarithmic scale for the current density. All measurements are conducted at room temperature. In the N-polar GaN sample, curve fitting using Equation (1) in the low-voltage region (<0.15 V but greater than 3kT/q) provides the barrier height (φₜₐ₈) of 0.58 V and an ideality factor (n) of 1.07. In contrast, the Ga-polar GaN sample exhibits the φₜₐ₈ and n of 0.79 V and 1.04, respectively, by curve fitting with the same voltage range. The results of the ideality factor suggest that the J–V characteristics are well expressed by Equation (1) in the fitting range. Nevertheless, the obtained barrier height in the N-polar GaN is smaller than that in the Ga-polar GaN by 0.21 V.

Figure 3 shows the typical (1/C²)–V characteristics obtained by the C–V measurements under the reverse bias condition for the N- and Ga-polar GaN samples. From the slope of the (1/C²)–V plots, the donor concentration (N_D) is estimated to be 1.5 × 10¹⁸ cm⁻³ for the N-polar GaN and 6.6 × 10¹⁶ cm⁻³ for the Ga-polar GaN sample. Although the N-polar GaN layer is unintentionally doped, the large N_D on the order of 10¹⁸ cm⁻³ occurs due to oxygen impurities incorporated during MOVPE growth. Reducing these impurities will be the focus of future work. The linear extrapolation value to the horizontal axis shown in Figure 3 provides ψₜₐ₈ = C/D from Equation (2). On the basis of this result, Equation (3) estimates the barrier height (φₜₐ₈) to be 0.83 and 1.04 V in the N-polar and Ga-polar GaN samples, respectively. The discrepancy of φₜₐ₈ obtained by the J–V and C–V measurements is a commonly observed phenomenon in nonideal Schottky diodes in which the barrier height deduced from J–V curves is expected to be smaller[12]. Again, the C–V characterization result indicates that the differences in φₜₐ₈ between the two polarizations is 0.21 V.

3.2. Model of Effective Schottky Barrier Height Affected by Polarization Charges

The differences in φₜₐ₈ obtained in this study and in earlier reports are shown in Table 1. In all cases, Ga-polar GaN exhibits a larger
\( \phi_B \), and the difference in \( \phi_B \) between the two polarities is in the range of 0.2–0.5 V. This polarity dependence of the Schottky barrier height seems to stem from the influence of polarization charges, in which the difference of \( \phi_B \) between N- and Ga-polar GaN can be explained by the different surface electron affinity. Specifically, the negative polarization charges at the surface of Ga-polar GaN cause a large band bending that reduces the electron affinity at the surface in comparison with that at the N-polar GaN surface.\(^{[12]} \) Because \( \phi_B \) is deduced by subtracting the electron affinity of the semiconductor from the work function of the metal, the reduction in the electron affinity results in an increase in \( \phi_B \). However, the electron affinity is the potential difference between the conduction band minimum and the vacuum level—and thus, in principle, is a material parameter—so it should be identical for GaN regardless of crystal orientation or impurity concentration. Nevertheless, the band bending caused by the polarization charges cannot be ignored because these charges are significantly large in GaN \((3.4 \times 10^{-6} \text{ C cm}^{-2})\), which corresponds to the sheet charges stemming from ionized impurities as large as \(2.12 \times 10^{13} \text{ cm}^{-2}\).
To clarify the band bending caused by the polarization charges, we propose the *polarization-induced surface charges with finite thickness* model. Conventional models assume that polarization charges are located at an infinitely thin plane on the surface of the GaN layer. In the following subsections, we numerically calculate the potential profile using both the conventional polarization surface charges model and our model.

### 3.2.1. Numerical Calculation of Band Profile

First, we calculate the band profile of GaN using Silvaco Atlas with a built-in polarization charge model (Figure 4). We find that the calculated band profile is completely the same between N-polar and Ga-polar GaN. The maximum of the conduction band energy is located at the surface, and its value is the same as the Schottky barrier height. In this model, the polarization charges (positive at N-face and negative at Ga-face) are located exactly at the surface with infinitely thin thickness. However, these polarization charges do not affect the band profile because the potential at the surface is defined by the given boundary condition (in the case of a Schottky contact, the boundary condition is defined by a given barrier height and an applied voltage). Therefore, we need to specify different values of Schottky barrier height for N- and Ga-polar GaN surfaces to accurately represent the experimental results. Next, we model the polarization charges by 3D fixed charges \( \rho \) uniformly distributed in the region with a thickness of \( \delta \) so that the sheet concentration of the charges becomes the same as the one calculated by the built-in polarization model, as shown in Figure 5. For Ga-polar GaN, a negative-charged region is located at the surface and a positive-charged region is located at the substrate interface, and vice versa for N-polar GaN. Figure 6 shows the calculation results for \( \delta \) of 5 and 10 Å. The calculated band profile for Ga-polar GaN exhibits a significant upward convex shape in the surface negative-charged region. As a result, the conduction band energy becomes largest at the bottom edge of the surface negative-charged region. Its maximum value should be regarded as the effective Schottky barrier height. For N-polar GaN, in contrast, the conduction band energy drastically decreases with increasing depth from surface in the surface positive-charged region. The resulting sharp wedge-shaped band profile at the surface positive-charged region may help electrons tunnel through this barrier. Therefore, we conclude the effective Schottky barrier height should be regarded as the energy at the bottom edge of the surface positive-charged region. The difference between the effective Schottky barrier height of Ga- and N-polar GaN increases with \( \delta \), becoming 0.18 and 0.38 eV at \( \delta \) of 5 and 10 Å, respectively.

### 3.2.2. Simple Analytical Model

The modification of Schottky barrier height by introducing a thin heavily doped layer at the semiconductor surface is known as a barrier-height adjustment. [16] One example of such adjustment is polarization surface charges with finite thickness. In GaN, the spontaneous polarization charges correspond to the charges stemming from impurities with a concentration of \( 4.25 \times 10^{20} \) and \( 2.125 \times 10^{20} \) cm\(^{-3} \) for \( \delta \) of 5 and 10 Å, respectively. These are significantly larger than the impurity concentration achieved by normal doping techniques. By solving a 1D Poisson equation for the charge distribution shown in Figure 7, the shift in...
the effective Schottky barrier height from its intrinsic value (Δϕ in Figure 7) is approximately given as follows if the doping concentration in the GaN layer is \(N_D\) and \(|\rho| \gg qN_D\):

\[
\Delta \phi = \frac{\rho \delta^2}{2\varepsilon_s} = -\frac{P\delta}{2\varepsilon_s} \tag{4}
\]

Equation (4) indicates that \(\Delta \phi\) is positive for the Ga-polar GaN surface \((P < 0)\) and negative for the N-polar GaN surface \((P > 0)\). The difference in the effective Schottky barrier height between Ga- and N-polar GaN is therefore \(2|\Delta \phi|\), which can be calculated to be 0.22 and 0.43 V for \(\delta\) of 5 and 10 Å, respectively. These values are fairly consistent with the numerical calculation results shown in Section 3.2.1 within an error of 0.05 V.

Figure 6. Calculated band profiles using polarization-charge layer thickness of 5 Å (left) and 10 Å (right). Insets: Magnification of the band profile near the surface.

(a) charge density (b) charge density

| \(\rho\) | \(qN_D\) | \(\delta\) | \(\rho\) | \(qN_D\) | \(\delta\) |
|---|---|---|---|---|---|
| energy | energy | \(q\phi_{Bi}\) | \(q\phi_{Bi}\) | \(\Delta \phi\) | \(\Delta \phi\) |

Figure 7. Charge profile (top) and band profile (bottom) of a) N-polar GaN and b) Ga-polar GaN.

We should emphasize here that the intrinsic Schottky barrier height (\(\phi_{Bi}\) in Figure 7) is identical for both N- and Ga-polar GaN. This is consistent with the fact that the electron affinity is unique in each material. This model also enables us to explicitly show the influence of the polarization charges on the band profile (as shown in the inset of Figure 6), whereas the overall shape of the band profile looks the same as conventionally accepted ones \(\text{i.e., a normal Schottky barrier shape with different barrier height for each polarity)}\ (Figure 6). The difference in the effective barrier height between N- and Ga-polar GaN can be determined by the thickness of the polarization-charge layer \(\delta\). Our experimental results indicate that the difference is 0.21 V, from which \(\delta\) is deduced to be about 5 Å. Interestingly, the obtained \(\delta\) is close to the height of the unit cell of wurtzite GaN along the \(c\)-axis. In wurtzite GaN crystal, as shown in Figure 8, the charge center of cations (Ga\(^+\)) is located at the center of the unit cell, whereas that of anions (N\(^-\)) are shifted toward the positive direction on the \(c\)-axis in each unit cell. Resulting dipoles make the unit cells negatively charged at the Ga-face boundary and positively charged at the N-face boundary. Inside a bulk crystal, however, the charges at the unit cell boundary are neutralized by the charges with an opposite sign originating in the neighboring unit cell. As a result, only the charges facing the edge of the crystal (i.e., the surface) become visible as the polarization charges. When we consider that the dipoles in unit cells are the origin of the polarization charges, a thickness of the polarization-charge layer \(\delta\) of less than or close to the unit cell height is reasonable.

We should point out, however, that the experimental conditions might contain other aspects that influence the barrier height difference between samples with two polarities. As discussed in the C–V measurement results, the N-polar sample contains a higher impurity concentration than the Ga-polar reference. In addition, the N-polar sample contains a higher dislocation density because the N-polar sample is grown on a SiC substrate, whereas the Ga-polar reference is grown on a freestanding GaN substrate. These differences in the sample quality...
could affect the evaluated barrier height and therefore result in an overestimated $\delta$. Our future work will involve a more exact determination of $\delta$ in which the characterization is done using N- and Ga-polar GaN with the same quality and same impurity concentration.

4. Conclusions

In this work, we modeled the difference in Schottky barrier height between N-polar and Ga-polar GaN by polarization-induced surface charges with finite thickness. The results suggest a unified understanding of the difference in effective Schottky barrier height of GaN with different polarities from a common intrinsic Schottky barrier height. From the experimental characterization of Schottky diodes, we estimate the difference in the effective Schottky barrier height to be 0.21 V and the thickness of the surface polarization layer to be 5 Å.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords

barrier height, gallium nitride, nitrogen-polar materials, polarization charges

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