# A simple method of extracting the polarization charge density in the AlGaN/GaN heterostructure from current–voltage and capacitance–voltage characteristics*

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An Ni Schottky contact on the AlGaN/GaN heterostructure is fabricated. The flat-band voltage for the Schottky contact on the AlGaN/GaN heterostructure is obtained from the forward current–voltage characteristics. With the measured capacitance–voltage curve and the flat-band voltage, the polarization charge density in the AlGaN/GaN heterostructure is investigated, and a simple formula for calculating the polarization charge density is obtained and analyzed. With the approach described in this paper, the obtained polarization charge density agrees well with the one calculated by self-consistently solving Schrodinger's and Poisson's equations.

**Keywords:** AlGaN/GaN heterostructures, flat-band voltage, polarization charge density

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## 1. Introduction

AlGaN/GaN heterostructure field-effect transistors (HFETs) exhibit excellent high frequency, high power, and high temperature performance and have the potential to replace Si- and GaAs-based transistors for a number of applications.[1,2] To improve the performance of the AlGaN/GaN devices, an accurate determination of the polarization charge density at the interface in the nitride heterostructure is essential. So far, the density of the polarization charge can be calculated theoretically based on the structural parameters of the AlGaN/GaN heterostructures.[3−5] However, the theoretical prediction for the polarization charge density is not accurate due to the influence caused by the later device processings, such as Ohmic contact metal annealing and Schottky contact metal deposition.[6,7] The precise measurement of the polarization charge density for the AlGaN/GaN heterostructure can be carried out with the capacitance–voltage ($C$–$V$) measurement, however this approach is suitable for the doped AlGaN/GaN heterostructures not for the undoped ones.[8] Moreover, when the Schottky barrier height of the AlGaN/GaN heterostructure is known, with the measured $C$–$V$ curve of the Schottky contacts on the AlGaN/GaN heterostructure, the density of the polarization charge can be accurately calculated by self-consistently solving Schrodinger's and Poisson's equations.[7] But this calculation is complicated, because with the self-consistent solution of Schrodinger's and Poisson's equations, the Schottky barrier height needs to be known. So far, few papers on directly and accurately extracting the polarization charge density in the AlGaN/GaN heterostructure have been published. Thus, it is necessary to find out a simple method of extracting the density of the polarization charge in the AlGaN/GaN heterostructure.

In this paper, with the prepared Ni Schottky contact on the AlGaN/GaN heterostructure, a simple method for extracting the polarization charge density in the AlGaN/GaN heterostructure from the forward current–voltage ($I$–$V$) characteristics has been analyzed and investigated.

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## 2. Experiment

The heterostucture layer employed in this study was epitaxially grown by metal organic chemical vapor deposition (MOCVD) on a (0001) sapphire substrate. The heterostructure layer consisted of a 40 nm AlN nucleation layer, followed by a 3 μm undoped GaN layer and a 21.5 nm undoped $Al_{0.3}Ga_{0.7}N$ barrier layer. Hall measurements indicated a sheet carrier density of around $1.36\times10^{13}$ cm$^{-2}$ and an electron mobility of 1200 cm$^2$/V·s at room temperature. The Ohmic contacts of Ti/Al/Mo/Au were fabricated by e-beam evaporation and lift-off. These contacts were annealed at 850 °C for 30 s in a rapid thermal annealing system. The diameter of the Ni/Au (60 nm/200 nm) circular Schottky contact was 120 μm. The separation between the Ohmic and the circular Schottky contacts was 20 μm. The $C$–$V$ measurement of the prepared Schottky contacts was performed by using an Aglient 4284A LCR meter, and a combination of a dc-biased voltage and an ac-modulation voltage of amplitude 0.1 V at the frequency of 10 kHz was applied between the Schottky and the Ohmic contacts. The photoemission measurement of the Schottky diode was performed with a halogen lamp as the light source, a monochromator (ISA, model HR-320), and a lock-in amplifier (EG&G, model 5209) for the photocurrent measurement. The $I$–$V$ measurement was performed using an Agilent 4156 semiconductor parameter analyzer.

## 3. Calculation and analyses

Figure 1 shows the measured forward $C$–$V$ curve of the prepared AlGaN/GaN Schottky diode. By the $C$–$V$ curve integration, the two dimensional electron gas (2DEG) sheet carrier density $n_{2D}$ under the Schottky contact metals at zero bias is calculated to be $9.732\times10^{12}$ cm$^{-2}$ for the diode.[9]

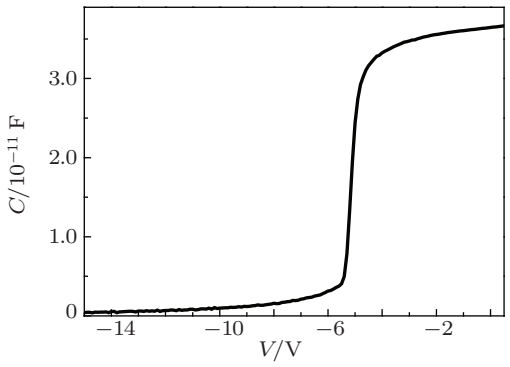



**Fig. 1.** Measured capacitance–voltage curve at room temperature with the frequency of 10 kHz for the Ni Schottky contact.

Figure 2 shows the measured forward $I$–$V$ curve of the diode, and the current of the shunt conduction path has been deducted from the measured $I$–$V$ curve.[10] Figure 3 shows the band diagram of the AlGaN/GaN heterostructure at zero bias, in which the bottom of the triangle quantum well is assumed to be zero. AlGaN/GaN diodes can be visualized as two diodes back-to-back in series (Fig. 3).[10] The left diode (diode 1) represents the Schottky contact between the Schottky metals and the AlGaN barrier layer. The right diode (diode 2) represents the effective Schottky contact between the 2DEG and the AlGaN barrier layer.[11] As shown in Fig. 2, by fitting two straight lines to the current curve, the flat-band voltage $V_0$ can be obtained.[12] According to Ref. [12], the relationship between the flat-band voltage $V_0$ and the Schottky barrier height at zero electric field $\phi_{BF}$ is

$$\phi_{BF} = \phi_{b2}(0) + V_0, \tag{1}$$

where $\phi_{b2}(0)$ is the Schottky barrier height of diode 2.

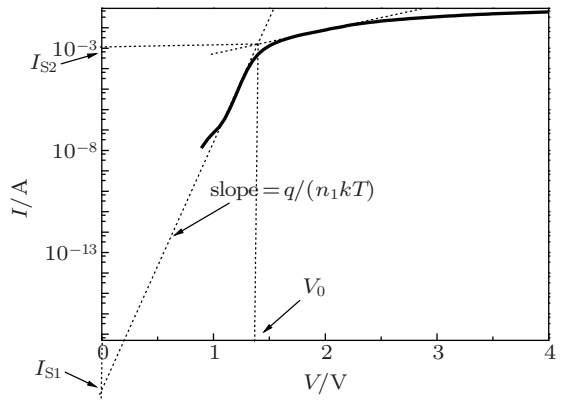



**Fig. 2.** Measured forward current–voltage curve for the Ni Schottky contact, with which the current of the shunt conduction path can be deducted.

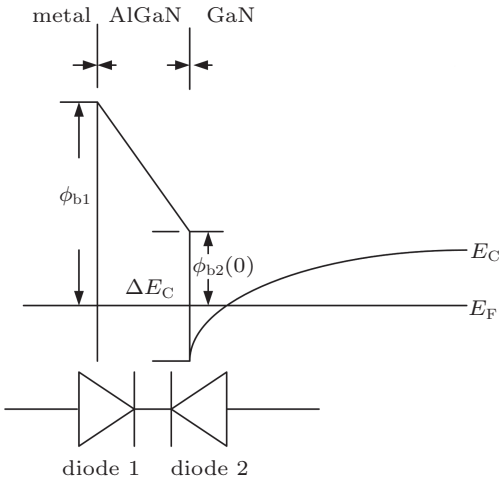



**Fig. 3.** Conduction band diagram of the AlGaN/GaN heterostructure at zero bias.

It is well known that the barrier height of a Schottky barrier diode is electric field dependent.[13] The relationship between the Schottky barrier height ($\phi_{b1}$) at zero bias and the one ($\phi_{BF}$) at zero electric field is[10]

$$\phi_{BF} = n_1\phi_{b1} - (n_1 - 1)\phi_{b2}(0), \tag{2}$$

where $n_1$ is the ideality factor of diode 1 and can be obtained from the slope of the first fitted straight dotline.[10] Substituting Eq. (1) into Eq. (2), we obtain the following expression

$$n_1 = V_0/(\phi_{b1} - \phi_{b2}(0)). \tag{3}$$

The polarization sheet charge density $\sigma$ at the AlGaN/GaN interface is given by[14]

$$q\sigma = qn_{2D} + \frac{\varepsilon_{AlGaN}\varepsilon_0}{d}(E_F + \phi_b - \Delta E_C), \tag{4}$$

where $\phi_b$ is the Schottky barrier height at zero bias and here is equal to $\phi_{b1}$, $\Delta E_C$ is the conduction-band offset and is calculated to be 0.42 eV for $Al_{0.3}Ga_{0.7}N/GaN$,[7] $E_F$ is the Fermi level in the AlGaN/GaN heterostructure at zero bias, $q$ is the electron charge, $\varepsilon_{AlGaN}$ is the value of the relative permittivity of the AlGaN barrier layer, $\varepsilon_0$ is the vacuum permittivity, and $d$ is the thickness of the AlGaN barrier layer. The relative permittivity of the AlGaN barrier layer $\varepsilon_{AlGaN}$ can be calculated by[15]

$$\varepsilon_{AlGaN} = \frac{Cd}{\varepsilon_0 S}, \tag{5}$$

where $S$ is the Ni Schottky contact area, and $C$ is the measured capacitance under zero bias between the Ohmic and the Schottky contacts. Substituting Eq. (5) into Eq. (4), we obtain the relationship between the polarization sheet charge density and the capacitance under zero bias

$$q\sigma = qn_{2D} + \frac{C}{S}(E_F + \phi_b - \Delta E_C). \tag{6}$$

As we can see from Fig. 3, the relationship between $\phi_{b2}(0)$ and $E_F$ is

$$\phi_{b2}(0) = \Delta E_C - E_F. \tag{7}$$

Substituting Eq. (7) into Eq. (6) yields the polarization sheet charge density $\sigma$

$$q\sigma = qn_{2D} + \frac{C}{S}(\phi_{b1} - \phi_{b2}(0)). \tag{8}$$

Substituting Eq. (3) into Eq. (8), we obtain a simple relationship between the polarization sheet charge density $\sigma$ and the flat-band voltage $V_0$

$$q\sigma = qn_{2D} + \frac{V_0 C}{n_1 S}. \tag{9}$$

The flat-band voltage $V_0$ and the ideality factor $n_1$ corresponding to our diode are determined to be 1.398 V and 1.351, respectively (as shown in Fig. 2). With the obtained values of $V_0$ and $n_1$, the polarization sheet charge density can be calculated with the measured $C$–$V$ curve and Eq. (9), and the value of the polarization sheet charge density for our diode is calculated to be $1.182\times10^{13}$ cm$^{-2}$.

As can be seen from Eq. (6), the polarization sheet charge density can also be calculated with the Schottky barrier height at zero bias and the Fermi level in the AlGaN/GaN heterostructure. The Fermi level can be obtained by self-consistently solving Schrodinger's and Poisson's equations.[7] According to Ref. [7], self-consistently solving Schrodinger's and Poisson's equations started with knowing the value of $\sigma$. However, by introducing

$$\sigma q n_{2DGaN} = \varepsilon_0\varepsilon_{GaN}E_2, \tag{10}$$

where $n_{2DGaN}$ is the 2DEG electron density in the GaN layer and is less than $n_{2D}$ due to the electron penetration into the AlGaN layer, $\varepsilon_{GaN}$ is the relative permittivity of the GaN layer and is 10.4,[4] and $E_2$ is the electric field in the GaN layer at the heterostructure interface, the self-consistent calculation can start without $\sigma$. The $n_{2DGaN}$ can be obtained by the following integration:

$$n_{2DGaN} = \int_{d_{AlGaN/GaN}}^{d_{GaN}} n(z)\,\mathrm{d}z, \tag{11}$$

where $z$ is the coordinate in a direction perpendicular to the AlGaN/GaN heterostructure with the origin at the surface of the AlGaN barrier layer, $n(z)$ is the electron concentration at point $z$, $d_{AlGaN/GaN}$ is equal to the value of $z$ at the AlGaN/GaN interface, and $d_{GaN}$ is the final value of $z$ in the GaN.

In the process of self-consistently solving Schrodinger's and Poisson's equations, $n_{2DGaN}$ is firstly assumed to be equal to $n_{2D}$. The $n(z)$ can be obtained by self-consistently solving Schrodinger's and Poisson's equations.[7] Then the new value of $n_{2DGaN}$ is obtained with Eq. (11). We then replace the initial $n_{2DGaN}$ by the new calculated one and iterate the above process until the difference between the latest and the prior $n_{2DGaN}$ values is less than a specified value.

Figure 4 shows the photocurrent spectrum of the Ni Schottky contact. The Schottky barrier height under zero electric field $\phi_{BF}$ can be obtained in the photoemission measurement,[10,16] the obtained $\phi_{BF}$ for

the prepared diode is 1.47 eV. With the obtained $\phi_{\rm BF}$, the Schottky barrier height at zero bias $\phi_{\rm b1}$ and the Fermi level $E_{\rm F}$ in the AlGaN/GaN heterostructure can be determined by the following iterative calculation.

The $\phi_{\rm b2}(0)$ is firstly assumed to be equal to a given value (0–1 eV or more). From Eq. (2), the value of $\phi_{\rm b1}$ can be obtained with the known values of $\phi_{\rm BF}$, $\phi_{\rm b2}(0)$, and $n_1$. With the obtained values of $n_{\rm 2D}$ and $\phi_{\rm b1}$, $E_{\rm F}$ at zero bias can be calculated by self-consistently solving Schrodinger's and Poisson's equations.[7] The new $\phi_{\rm b2}(0)$ is obtained with Eq. (7). We then replace the initial $\phi_{\rm b2}(0)$ by the new calculated one and iterate the above process until the difference between the latest and the prior $\phi_{\rm b2}(0)$ values is less than a specified value. With this iterative calculation, $\phi_{\rm b1}$, $E_{\rm F}$, and $\phi_{\rm b2}(0)$ can be determined, and they are 1.12 eV, 0.316 eV, and 0.104 eV, respectively. Thus, from Eq. (6), the polarization sheet charge density can be calculated with the obtained values of $\phi_{\rm b1}$ and $E_{\rm F}$, and the value of the polarization sheet charge density is calculated to be $1.178\times10^{13}$ cm$^{-2}$.

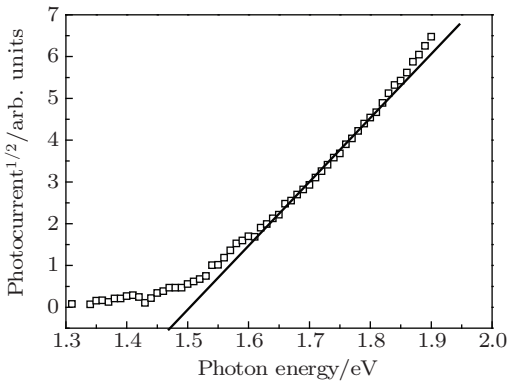



**Fig. 4.** Photoemission spectrum of the Ni Schottky contact.

As can be seen, the polarization sheet charge density ($1.182\times10^{13}$ cm$^{-2}$) calculated with the forward $I$–$V$ characteristics by Eq. (9) agrees well with the one ($1.178\times10^{13}$ cm$^{-2}$) obtained by Eq. (6) with self-consistently solving Schrodinger's and Poisson's equations. Therefore, it is shown that the method of extracting the density of the polarization charge in the AlGaN/GaN heterostructure from the forward $I$–$V$ characteristics is feasible. Comparing Eq. (9) with Eq. (6), we note that the approach described in this paper does not involve the Schottky barrier height and the self-consistent solution of Schrodinger's and Poisson's equations, as a result, the approach with the forward $I$–$V$ characteristics for extracting the polarization charge density in the AlGaN/GaN heterostructure is simpler and more universal.

# 4. Conclusion

In summary, with the prepared Ni Schottky contact on the AlGaN/GaN heterostructure and based on the measured $I$–$V$ and $C$–$V$ characteristics for the AlGaN/GaN Schottky diode, a simple calculating formula for the polarization charge density in the AlGaN/GaN heterostructure has been obtained and analyzed, and the parameters involved in the calculating formula can be easily obtained from the measured $C$–$V$ and forward $I$–$V$ characteristics. The polarization charge density obtained with this simple calculating formula is in good agreement with the one calculated by self-consistently solving Schrodinger's and Poisson's equations. Thus, a simple method of extracting the polarization charge density in the AlGaN/GaN heterostructure is developed.

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