Different influences of Schottky metal on the strain and relative permittivity of barrier layer between AlN/GaN and AlGaN/GaN heterostructure Schottky diodes*

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Ni/Au Schottky contacts on AlN/GaN and AlGaN/GaN heterostructures are fabricated. Based on the measured current–voltage and capacitance-voltage curves, the polarization sheet charge density and relative permittivity are analyzed and calculated by self-consistently solving Schrödinger's and Poisson's equations. It is found that the values of relative permittivity and polarization sheet charge density of AlN/GaN diode are both much smaller than the ones of AlGaN/GaN diode, and also much lower than the theoretical values. Moreover, by fitting the measured forward *I*–*V* curves, the extracted dislocations existing in the barrier layer of the AlN/GaN diode are found to be much more than those of the AlGaN/GaN diode. As a result, the conclusion can be made that compared with AlGaN/GaN diode the Schottky metal has an enhanced influence on the strain of the extremely thinner AlN barrier layer, which is attributed to the more dislocations.

Keywords: Al(Ga)N/GaN, strain, relative permittivity, Schottky metal

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1. Introduction

The AlN/GaN heterostructure is an attractive material system for high frequency field-effect transistor (FET) devices due to the high polarization difference between the AlN barrier and the GaN buffer layer. Two-dimensional electron gas (2DEG) densities of up to 6×10^{13} cm^{-2} can be reached and planar enhancement mode devices have been realized.[1–3] Due to the thin barrier layer and polarization effects, AlN/GaN HEMT with an increased drain-to-source distance of 70 nm demonstrates a record-high $f_{\rm T}/f_{\rm max}$ of 342 GHz/518 GHz.[4] Furthermore, due to the interaction between the atoms of the Schottky metal and the surface atoms of Al(Ga)N barrier layer, the Schottky metal has an influence on the strain of barrier layer,[5] which further affects the device performance and reliability. Moreover, the converse piezoelectric effect in the AlN/GaN HFET is proportional to the relative permittivity of the barrier layer,[6,7] which also affects the device working reliability. However, so far little attention has been paid to the strain and relative permittivity of AlN layer in the AlN/GaN HFET. Thus, it is of great importance to investigate the influences of Schottky metal on the strain and relative permittivity of AlN barrier layer in AlN/GaN diode. Since the AlN/GaN and AlGaN/GaN heterostructures are both main-stream materials for microwave devices and digital circuits,[8] a comparison of the influence of Schottky metal on the strain and relative permittivity of barrier layer between AlN/GaN diode and AlGaN/GaN diodes is of great importance to further improve the performance and reliability of GaN-based frequency devices and the digital circuit.

In this paper, Ni/Au Schottky contacts on AlN/GaN and AlGaN/GaN heterostructures are prepared, respectively. Based on the measured current–voltage (*I*–*V*) curves and the capacitance–voltage (*C*–*V*) curves, the Schottky barrier height, relative permittivity, and polarization sheet charge density of each sample are analyzed and compared by self-consistently solving Schrödinger's and Poisson's equations. Moreover, the dislocation densities (DDs) existing in the barrier layer are extracted by fitting the dislocation-governed tunneling to the measured *I*–*V* curves. It is found that the influences of Schottky metal on the strain and relative permittivity of barrier layer in the AlN/GaN diode are different from those in the AlGaN/GaN diode.

2. Experiment

The AlN/GaN and AlGaN/GaN heterostuctures employed in this work are both epitaxially grown by metal–organic chemical vapor deposition (MOCVD) on a (0001) sapphire substrate. The AlN/GaN heterostructure consists of a low-temperature nucleation layer, followed by a 2-μm S. I. GaN, a 3-nm AlN barrier layer, and a 1-nm S. I. GaN cap. Hall measurements indicate a sheet carrier density of around 1.05×10^{13} cm^{-2} and an electron mobility of 1650 cm^2/V·s at

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room temperature. The AlGaN/GaN heterostructure consists of a low-temperature nucleation layer, followed by a 2-μm S. I. GaN, a 1-nm AlN interlayer, and finally a 22.5-nm thick undoped $Al_{0.3}Ga_{0.7}N$ barrier layer. Hall measurements indicate a sheet carrier density of around 1.07×10^{13} cm^{-2} and an electron mobility of 1800 cm^2/V·s at room temperature. Uniform device processing is performed on the two different heterostructures. Ohmic contacts of Ti/Al/Ni/Au are fabricated by e-beam evaporation and lift-off. The Ohmic contacts consist of a ring with an inner diameter of 600 μm and an outer diameter of 650 μm. A rapid thermal annealing is taken to form good Ohmic contacts. With transmission line method (TLM) patterns, the specific resistivities of the Ohmic contacts for AlN/GaN and AlGaN/GaN diodes are measured to be 5.1×10^{-5} Ω·cm^2 and 5.9×10^{-5} Ω·cm^2, respectively. Ni/Au (50 nm/200 nm) circular Schottky contacts each with a diameter of 300 μm are finally deposited by e-beam evaporation. *C–V* measurements are performed at room temperature using an Agilent B1520A at different frequencies of 10 kHz, 100 kHz, and 1 MHz. The *I–V* characteristics are measured at room temperature using Keithley 4200 semiconductor parameter analyzer.

3. Calculation and analysis

Figures 1(a) and 1(b) show the measured *C–V* curves under different frequencies of 10 kHz, 100 kHz, and 1 MHz for AlN/GaN and AlGaN/GaN Schottky diodes, respectively. For both AlN/GaN and AlGaN/GaN Schottky diodes, the measured *C–V* curves under frequencies of 10 kHz and 100 kHz are almost the same; however, the one under a frequency of 1 MHz is much lower. This may be induced by the deep level defects, which needs further investigation. The two-dimensional electron gas (2DEG) electron density (n_{2D}) under zero gate bias of the Schottky diode can be obtained by integrating the measured *C–V* curve[9]

$$n_{2D} = \int_{V_T}^{0} \frac{C\,\mathrm{d}V}{(Sq)}, \tag{1}$$

where C is the measured capacitance between the Ohmic contact and the Ni Schottky contact, V_T is the threshold voltage and can also be obtained by the *C–V* curve integration (inserted in Fig. 1),[9] and S is the Ni Schottky contact area. Using the measured *C–V* curve under a frequency of 1 MHz, the 2DEG electron densities under zero gate bias for AlN/GaN and AlGaN/GaN Schottky diodes are calculated to be 5.72×10^{12} cm^{-2} and 8.86×10^{12} cm^{-2}, respectively.

The polarization sheet charge density (σ) at the Al(Ga)N/GaN interface is given by[10]

$$\frac{q(\sigma - n_{2D})}{(E_F + \phi_b - \Delta E_C)} = \frac{\varepsilon_{Al(Ga)N}\varepsilon_0}{d}, \tag{2}$$

where E_F is the Fermi level in the Al(Ga)N/GaN heterostructures, ϕ_b is the Schottky barrier height under zero gate bias, ΔE_C is the conduction-band offset,[11] ε_0 is the vacuum permittivity, d is the thickness of the Al(Ga)N barrier layer, and $\varepsilon_{Al(Ga)N}$ is the relative permittivity of the Al(Ga)N barrier layer, which can be obtained by using the measured *C–V* characteristics[7,12]

$$\varepsilon_{Al(Ga)N} = \frac{Cd}{\varepsilon_0 S}. \tag{3}$$

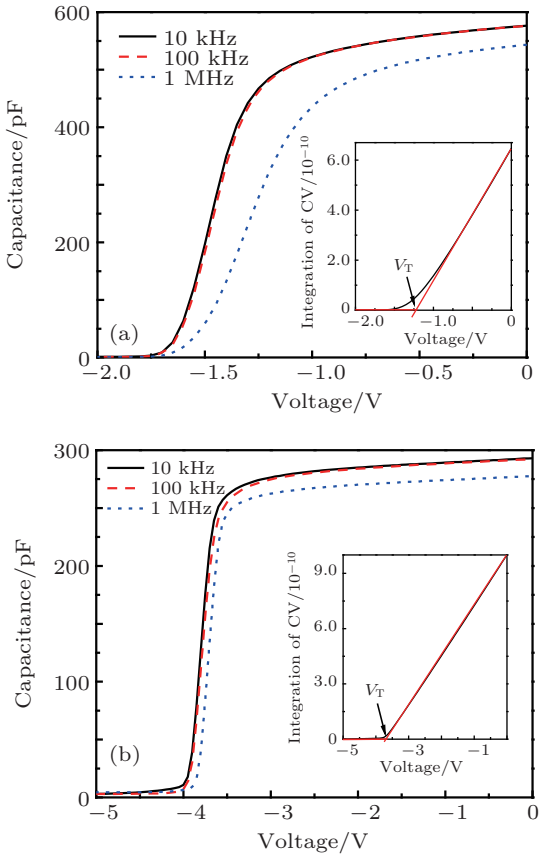


Fig. 1. (color online) Measured *C–V* curves under different frequencies of 10 kHz, 100 kHz, and 1 MHz for the prepared AlN/GaN (a) and AlGaN/GaN (b) Schottky diodes.

Additionally, Ambacher *et al.*[13] reported that the relationship between relative permittivity ($\varepsilon_{Al(Ga)N}$) and the Al concentration (x) obeys[13]

$$\varepsilon_{Al_xGa_{1-x}N} = 10.4 - 0.3x. \tag{4}$$

With Eqs. (3) and (4), the relative permittivities for both AlN/GaN and AlGaN/GaN Schottky diodes are calculated, and the results are summarized in Table 1. It is found that the relative permittivity (10) of AlGaN/GaN heterostructure obtained from *C–V* curve is almost consistent with the theoretical one (10.31) from Eq. (4). However, the relative permittivity (4.3) of AlN/GaN heterostructure obtained by the *C–V* curve is much smaller than the theoretical one (10.1).

The Fermi level (E_F) and the Schottky barrier height under the zero gate bias (ϕ_b) can be obtained by self-consistently solving Schrödinger's and Poisson's equations as follows.[14,15]

According to Chen *et al.*'s two-diode model,[16] an Al(Ga)N/GaN structure consisting of a Schottky metal can be considered as two diodes connected in series back to back (shown in Fig. 2). The first diode (diode 1) represents the Schottky contact between the Schottky metal and the Al(Ga)N barrier layer, and the second diode (diode 2) represents the effective Schottky contact between the Al(Ga)N barrier layer and the 2DEG.[15,16]

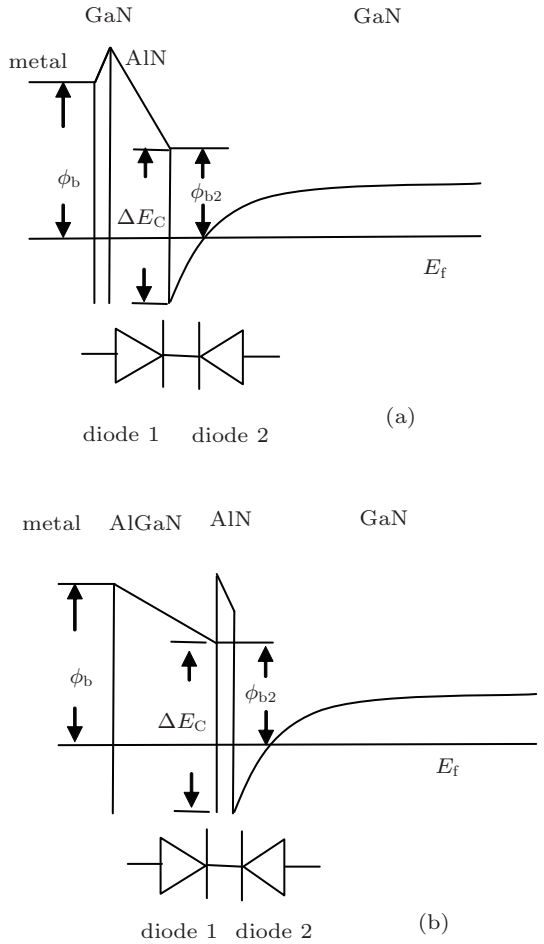


Fig. 2. Conduction band diagrams of the AlN/GaN (a) and AlGaN/GaN (b) heterostructure at zero bias and the two-diode equivalent circuit.

Figures 3(a) and 3(b) show the measured forward *I*–*V* curves of AlN/GaN and AlGaN/GaN Schottky diodes at room temperature, respectively. According to the two-diode model the flat-band voltage (V_0) can be determined by fitting two straight lines to the measured forward *I*–*V* curve (shown in Fig. 3). The relationship between Schottky barrier height under zero electric field (ϕ_{BF}) and the flat-band voltage is given by[14]

$$\phi_{BF} = V_0 + \phi_{b2}, \tag{5}$$

where ϕ_{b2} is the effective Schottky barrier height of diode 2 (shown in Fig. 2). The relationship between the Schottky barrier height (ϕ_b) at zero bias and the one (ϕ_{BF}) at zero electric field is given by[14]

$$\phi_{BF} = n_1\phi_b - (n_1 - 1)\phi_{b2}, \tag{6}$$

where n_1 is the ideality factor of diode 1 and can be obtained from the slope of *I*–*V* curve.[15] Thus, based on the obtained 2DEG electron density and flat-band voltage, the Schottky barrier height of the AlN/GaN or AlGaN/GaN Schottky diode can be calculated by self-consistently solving Schrödinger's and Poisson's equations.[14,15] The details of the above calculation can refer to Ref. [15]. The calculated results are shown in Table 1. It is found that the calculated Schottky barrier height at zero electric field of AlN/GaN Schottky diode is higher than that of the AlGaN/GaN diode, which may be due to the larger bandgap of AlN.

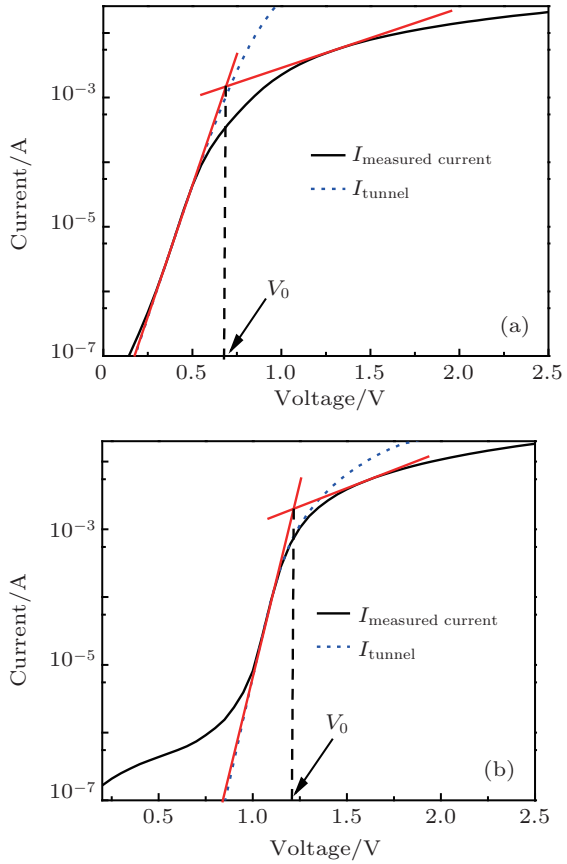


Fig. 3. (color online) Measured forward *I*–*V* curves of the prepared AlN/GaN (a) and AlGaN/GaN (b) Schottky diodes, respectively.

Based on the calculated values of Fermi level (E_F), Schottky barrier height (ϕ_b) and relative permittivity ($\varepsilon_{Al(Ga)N}$), the polarization sheet charge density (σ) at the Al(Ga)N/GaN interface can be obtained from Eq. (2), and the results are summarized in Table 1.

As seen from Table 1, the calculated 2DEG density of the AlN/GaN diode is much smaller than the Hall measurement. Moreover, it is well known that the polarization of

$Al_xGa_{1-x}N$ barrier layer increases as the Al concentration (x) increases.[13] However, the calculated polarization density of AlN/GaN diode is abnormally much smaller that of the AlGaN/GaN diode. To explain the abnormal behaviors of relative permittivity and polarization for AlN/GaN diode, DD is calculated as follows.

Table 1. Calculated values of 2DEG electron density, relative permittivity, Schottky barrier height, Fermi level, and polarization sheet charge density for AlN/GaN and AlGaN/GaN Schottky diodes.

	n_{2D}/cm^{-2}	$\varepsilon_{Al(Ga)N}$		ϕ_{BF}/eV	ϕ_b/eV	E_F/eV	σ/cm^{-2}
		C–V	Theoretical				
AlN/GaN	5.72×10^{12}	4.3	10.1	2.08	1.65	0.60	7.41×10^{12}
AlGaN/GaN	8.86×10^{12}	10	10.31	1.60	1.15	0.55	1.20×10^{13}

The tunneling current (I_{tunnel}) through the Al(Ga)N barrier is given by[17,18]

$$I_{tunnel} = I_t \left\{ \exp\left[\frac{q(V - IR_S)}{E_0} \right] - 1 \right\}, \tag{7}$$

where I_t is the tunneling saturation current, E_0 is the tunneling parameter, R_S is the series resistance and can be obtained by the plot of $d(V)/d(\ln I)$ versus I.[19] Taking the I_t and E_0 as adjustable fit parameters, we fit the experimental I–V data to the analytical expression (7). As shown in Fig. 3, it is found that the measured I–V data and the dislocation-governed tunneling expression are in excellent agreement for both AlN/GaN and AlGaN/GaN Schottky diodes. The tunneling saturation current (I_t) can be represented by the equation of the form[17]

$$I_t = qD\upsilon_D \exp(-qV_K/E_0), \tag{8}$$

where D is the dislocation density, υ_D is the Debye frequency, and V_K is the diffusion potential for the Schottky barrier diode. By using $\upsilon_D = 1.68\times10^{13}$ s^{-1}, $V_K = 1.15$ eV for both AlN/GaN and AlGaN/GaN diodes, and the determined $I_t(0)$ and E_0 from the measured I–V characteristic, the DDs of AlN/GaN and AlGaN/GaN diodes are obtained and summarized in Table 2. The details of the calculation can refer to Ref. [18]. Due to the larger Schottky barrier height, the value of V_K of the AlN/GaN diode is larger that of the AlGaN/GaN diode. However, even using the same value of V_K the calculated DD of AlN/GaN diode is much larger than the one of AlGaN/GaN diode (Table 2). Thus, the abnormal behaviors of relative permittivity and polarization for AlN/GaN diode can be explained in the following.

Table 2. Calculated values of tunneling saturation current, tunneling parameter, dislocation density, and ideal factor for AlN/GaN and AlGaN/GaN Schottky diodes.

	$I_t(0)$/(A/cm^2)	E_0/eV	D/cm^{-2}	n_1
AlN/GaN	3.77×10^{-6}	0.053	3.7×10^{9}	2.16
AlGaN/GaN	7.56×10^{-14}	0.032	5.5×10^{8}	1.57

When Schottky contact metal is deposited on the strained Al(Ga)N/GaN heterostructure, there appears an interaction between the atoms of Schottky contact metals and surface atoms of Al(Ga)N barrier layer.[5,20] During the interaction, the energy of the Al(Ga)N barrier layer will be changed, resulting in a strain energy variation in the Al(Ga)N barrier layer. Since there are only several atom layers in the extreme thin barrier layer ($\sim$ 3 nm), the interaction will induce larger strain variation in the AlN/GaN heterostructure. In addition, the existing defects in the barrier layer aggravate the interaction between Schottky contact metals and Al(Ga)N barrier layer.[21] The larger dislocation density for AlN/GaN diode further enhances the strain variation induced by the Schottky metal. Thus, due to more defects in the thinner barrier layer, the Schottky metal has a greater influence on the strain of the barrier layer for the AlN/GaN diode than for the AlGaN/GaN diode. The enhanced influence results in the fact that the AlN/GaN diode suffers much smaller polarization and relative permittivity than AlGaN/GaN diode. Besides, the existing theoretical expressions for the polarization and relative permittivity with Al concentration are not suitable for extremely thin-barrier AlN/GaN heterostructure and need further experimental and theoretical study.

4. Conclusion

In this paper, Ni/Au Schottky contacts on AlN/GaN and AlGaN/GaN heterostructures are fabricated. The DD existing in the barrier layer is extracted by fitting the dislocation-governed tunneling equation to the measured I–V curves. It is found that the DD of the AlN/GaN diode is much larger than that of the AlGaN/GaN diode due to the larger mismatch. Based on the measured current–voltage (I–V) curves and the capacitance–voltage (C–V) curves, the 2DEG electron density, the Schottky barrier height, the relative permittivity, and the polarization sheet charge density of each sample are calculated and compared by self-consistently solving Schrödinger's and Poisson's equations. It is found that, compared with AlGaN/GaN diode, the Schottky metal has an enhanced influence on the strain of the extremely thin AlN barrier layer, which is attributed to more dislocations. The enhanced influence of Schottky metal results in the fact that the AlN/GaN diode suffers smaller 2DEG electron density, weaker polariza-

tion, and lower relative permittivity.

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