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Determination of the relative permittivity of the AlGaN barrier layer in strained AlGaN/GaN heterostructures*

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Using the measured capacitance–voltage curves and the photocurrent spectrum obtained from the Ni Schottky contact on a strained $Al_{0.3}Ga_{0.7}N$/GaN heterostructure, the value of the relative permittivity of the AlGaN barrier layer was analysed and calculated by self-consistently solving Schrödinger's and Poisson's equations. It is shown that the calculated values of the relative permittivity are different from those formerly reported, and reverse biasing the Ni Schottky contact has an influence on the value of the relative permittivity. As the reverse bias increases from 0 V to –3 V, the value of the relative permittivity decreases from 7.184 to 7.093.

Keywords: relative permittivity, AlGaN barrier layer, AlGaN/GaN heterostructures
PACC: 7280E, 7360L

1. Introduction

A precise determination of the relative permittivity of the AlGaN barrier layer in strained AlGaN/GaN heterostructures is important for AlGaN/GaN heterostructure field effect transistors (AlGaN/GaN HFETs), because the relative permittivity is closely related to the polarization charge density of strained AlGaN/GaN heterostructures. So far, there have been several methods reported to calculate the relative permittivity of the AlGaN barrier layer, such as[1] $\varepsilon = 9.5 - 0.5x$, where ε is the relative permittivity of the AlGaN barrier layer and x is the Al content. Moreover, the relative permittivity has also been calculated by using the capacitance–voltage (C–V) characteristics of Schottky contacts on strained AlGaN/GaN heterostructures:[2] $C = \varepsilon_0\varepsilon S/d$, where ε_0 is the vacuum permittivity, C is the measured zero-biased capacitance value for Schottky contacts on strained AlGaN/GaN heterostructures, S is the Schottky contact area, and d is the thickness of the AlGaN barrier layer. Using the above different methods, the calculated values for the relative permittivity of the AlGaN barrier layer result in substantially different values. Therefore, it is necessary to find a method to determine the precise value of the relative permittivity of the AlGaN barrier layer.

In the work reported here, Ni Schottky contacts were deposited on strained AlGaN/GaN heterostructures, and capacitance–voltage and photoemission measurements were performed for the Ni Schottky contact. Schrödinger's equation and Poisson's equation were solved self-consistently for the strained AlGaN/GaN heterostructures. Combining the measured results with the self-consistently solved results, we precisely calculate the relative permittivity of the AlGaN barrier layer. In addition, we also study the influence of a reverse bias applied to the Schottky contact on

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the relative permittivity of the AlGaN barrier layer.

2. Experiments

The heterostructure employed in this study was epitaxially grown by metalorganic chemical vapour deposition (MOCVD) on a (0001) sapphire substrate. First a 40 nm AlN nucleation layer was grown, followed by a 3 μm undoped GaN and a 21.5 nm thick undoped $Al_{0.3}Ga_{0.7}N$ barrier layer. Hall measurements indicate a sheet carrier density of around 1.36×10^{13} cm^{-2} and an electron mobility of 1200 cm^2/(V·s) at room temperature. For device processing, the heterostructure wafers were first cleaned with organic solvents and blown dry with N_2, then the photolithographic technique was used to form an ohmic contact configuration. To remove the native oxide, the samples were dipped in an HCl:H_2O (1:2) solution for 30s, rinsed in deionized water for another 30s, and then blown dry with N_2. Immediately, the samples were loaded into an e-beam evaporator. Ohmic contacts of Ti/Al/Mo/Au (35 nm/90 nm/60 nm/100 nm) were evaporated on the AlGaN/GaN surface and then were lifted off in acetone. These contacts were annealed at 850 °C for 30s in an N_2 ambient in a rapid thermal annealing system. After forming a Schottky contact configuration by the photolithographic technique, the samples were also dipped in an HCl:H_2O (1:2) solution for 30s, rinsed in deionized water for another 30s, and blown dry with N_2, then they were immediately transferred to the e-beam evaporator. Ni/Au (60 nm/200 nm) circular Schotty contacts with a diameter of 120 μm were then formed by conventional e-beam evaporation and lift-off techniques. The separation between the ohmic contact and the circular Schottky contact was 40 μm. The C–V measurements were performed by using an Aglient 4284A LCR meter, and a combination of an ac-modulation voltage with an amplitude of ±0.1 V at frequencies of 1 kHz, 100 kHz, and 1000 kHz, respectively, and a dc-biased voltage was applied between the Schottky and ohmic contacts. The photoemission measurement was performed with a monochromator (ISA, model HR-320) and a lock-in amplifier (EG&G, model 5209) using a halogen lamp as a light source.

3. Calculations and discussions

Figure 1 shows the reverse biased conduction band diagram of the Ni Schottky contact on a strained AlGaN/GaN heterostructure, in which V is the reverse bias and $q\Phi_{\rm B}$ is the barrier height of the Schottky contact. $E_{\rm Fs}$ and $E_{\rm Fm}$ are the Fermi levels of semiconductor GaN and Schottky metals, respectively. When a small bias ΔV is added to the voltage, one part (ΔV_1) of the ΔV drops across the AlGaN barrier layer, the other (ΔV_2) is on the triangular quantum well. The conduction band diagram changes with the added ΔV bias (Fig.1 dash lines), and the electronic charge Q of the two dimensional electron gas (2DEG) also changes.

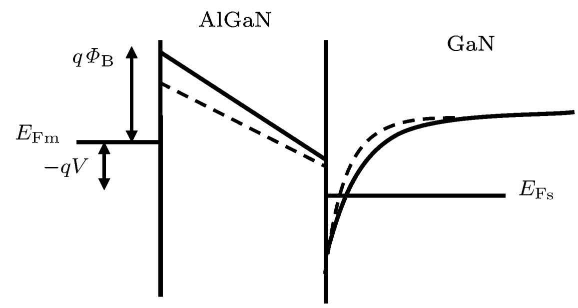

Fig.1. The reverse biased conduction band diagram of the Ni Schottky contact on strained AlGaN/GaN heterostructures.

The capacitance (C) of the Schottky contact on the strained AlGaN/GaN heterostructure can be calculated using

$$\begin{aligned} C &= \frac{\Delta Q}{\Delta V}, \\ \Delta V &= \Delta V_1 + \Delta V_2, \\ C &= \frac{1}{\dfrac{\Delta V_1}{\Delta Q} + \dfrac{\Delta V_2}{\Delta Q}}, \\ C &= \frac{1}{\dfrac{1}{C_1} + \dfrac{1}{C_2}}. \end{aligned} \tag{1}$$

ΔQ is the corresponding value of the 2DEG electronic charge with the applied bias ΔV. C_1 represents the capacitance value of the AlGaN barrier layer and can be written as

$$C_1 = \frac{\varepsilon_0 \varepsilon S}{d}. \tag{2}$$

The denotation of the symbols in Eq.(2) is the same as above. C_2 is the capacitance value of the 2DEG electrons in the triangular quantum well. By solving Schrödinger's and Poisson's equations self-consistently, the conduction band of the Schottky contact on strained AlGaN/GaN heterostructures (Fig.1) corresponding to reverse biased V and $V+\Delta V$ can be calculated and obtained. As a result, ΔV_2 is obtained, and ΔQ can be calculated by

$$\Delta Q = C\Delta V. \tag{3}$$

C is the measured capacitance value at reverse bias V, hence, the capacitance value of C_2 ($C_2 = \Delta Q/\Delta V_2$) is obtained. Since the capacitance values of C and C_2 are known, the capacitance value of C_1 can easily be calculated using Eq.(1), and the relative permittivity of the AlGaN barrier layer is also obtained using Eq.(2).

Figure 2 shows the photocurrent spectrum of the Ni Schottky contact. According to Fowler's theory,[3] the relationship between the photocurrent per photon, R, and the incident photon energy $h\nu$ is given by[3,4]

$$R \sim (h\nu - q\Phi_{\rm B})^2. \tag{4}$$

This relation is valid when $h\nu - q\Phi_{\rm B} > 3kT$. Therefore, the Schottky barrier can be obtained from the linear relationship of the square root of the photocurrent per photon versus the incident photon energy. Using photoemission measurements, the Schottky barrier height of the Ni Schottky contact on strained AlGaN/GaN heterostructures is determined to be 1.47 eV. It should be indicated that the deep levels inside the band gap of the semiconductor may have a contribution to the photocurrent[5] as an incident photon energy $h\nu$ larger than about 1.75eV, which results in rapid increase of the measured photocurrent in Fig.2.

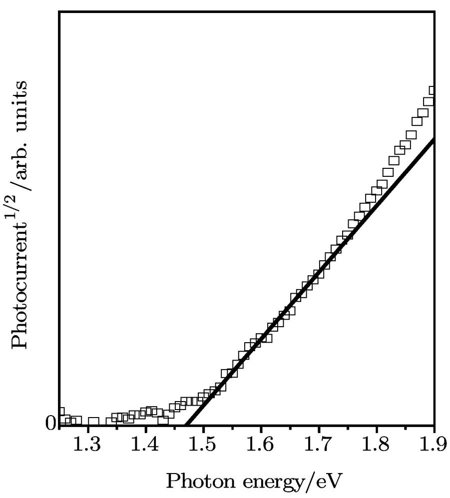

Fig.2. The measured photocurrent spectrum of the Ni Schottky contact.

Figure 3(a) shows the C–V curves of the Ni Schottky contact with measured frequencies of 1 kHz, 100 kHz and 1000 kHz. From the C–V curves with the different frequencies, it is found that there are trap charges in the AlGaN/GaN heterostructure. In order to remove the influence of the trap charges, the C–V curve with a frequency of 1000 kHz was used to calculate the relative permittivity of the AlGaN barrier layer. Integrating the C–V data yields the charge within the 2DEG versus voltage,[6] and the threshold voltage for the Ni Schottky contact is then obtained by linear extrapolation,[7] as shown in Fig.3(b). The

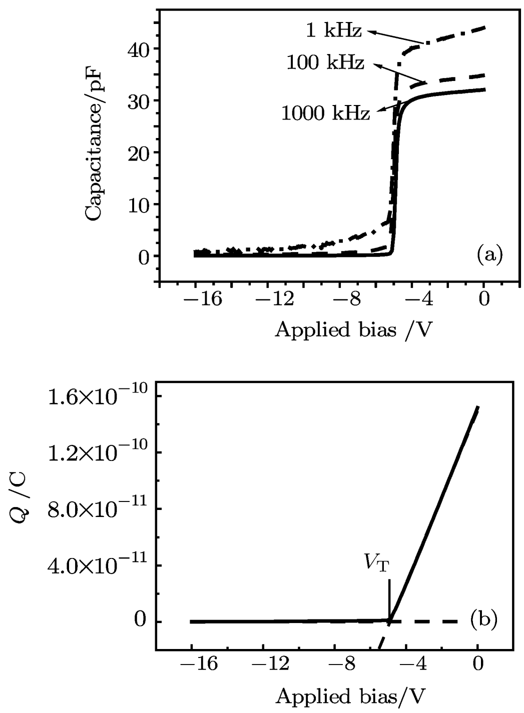

Fig.3. (a) The measured C–V curves with different frequencies at room temperature for the Ni Schottky contact, and (b) the charge Q in the two-dimensional channel of the strained AlGaN /GaN heterostructure, obtained by integration of the C–V curve with 1000 kHz in (a).

threshold voltage is –4.9 V for the Ni Schottky contact. The 2DEG electron density $n_{\rm 2D}$ under different biases can be calculated using

$$n_{\rm 2D} = \int_{V_{\rm T}}^{V} \frac{C{\rm d}V}{(Sq)}, \tag{5}$$

where q is the electron charge, C is the measured capacitance between the ohmic contact and the Ni Schottky contact, V is the applied bias, $V_{\rm T}$ is the threshold voltage, and S is the Ni Schottky contact area. What should be mentioned is that the 2DEG density calculated by the integration of the C–V curves ($\sim 8.26 \times 10^{12}$ cm^{-2}) is less than the

Hall measured result ($\sim 1.36 \times 10^{13}$ cm^{-2}). This difference can be attributed to the fact that when the Ni Schottky contact is deposited on the strained AlGaN/GaN heterostructure, some 2DEG electrons under the Ni Schottky contact are extracted to the void surface donor states[8] and therefore the 2DEG density is decreased.

The band gap of $Al_xGa_{1-x}N$ at room temperature is given by[9]

$$E_{\mathrm{g}}(x) = 6.13x + 3.42(1-x) - x(1-x) \qquad (6)$$

and the conduction-band offset is[10,11]

$$\Delta E_{\mathrm{c}} = 0.7[E_{\mathrm{g}}(x) - E_{\mathrm{g}}(0)]. \qquad (7)$$

In the calculation of Eqs.(6) and (7), the Al content is taken as 0.3, and ΔE_{c} is calculated as 0.42 eV. Based on the above equations and data, self-consistent solutions of Schrödinger's and Poisson's equations are performed.[12] In the calculation, 0.1 V (ΔV) is the applied AC bias, and the n_{2D} of different biases is calculated using Eq.(5). The results of the self-consistent solutions of Schrödinger's and Poisson's equations are listed in Table 1.

Table 1. The results of the self-consistent solutions of Schrödinger's and Poisson's equations.

applied biases/V	ΔV_1/V	ΔV_2/V	ΔQ/C
0	0.0958	0.0042	3.2037×10^{-12}
–1	0.0953	0.0047	3.1729×10^{-12}
–2	0.0948	0.0052	3.1424×10^{-12}
–3	0.0939	0.0061	3.1×10^{-12}

Using Eq.(1) and combining the calculated results (Table 1) with the measured C–V data (Fig.3(a)), the relative permittivity of the AlGaN barrier layer at different biases is obtained, as shown in Fig.4 (solid line). The dashed line in Fig.4 corresponding to the values of the relative permittivity of the AlGaN barrier layer is directly obtained by

$$C = \frac{\varepsilon_0 \varepsilon S}{d}, \qquad (8)$$

C is the measured capacitance value for the Ni Schottky contact (Fig.3(a)) at different biases and is the same as C_1, i.e. the capacitance of the 2DEG electrons in the triangular quantum well is ignored. It is found that the values of the relative permittivity calculated by Eq.(1) are different from those reported in the literature;[1,2] the values of the relative permittivity of the $Al_{0.3}Ga_{0.7}N$ barrier layer calculated in these papers are 9.35[1] and 6.88,[2] respectively. The relative permittivity calculated with $\varepsilon = 9.5 - 0.5x$[1] is determined by the Al-content x of the $Al_xGa_{1-x}N$ barrier layer, and it is obtained by linear interpolation between the tensor components of the relative permittivity of GaN and AlN on the {0001} basal plane. Because the device processing, such as ohmic contacts and Schottky contacts on strained AlGaN/GaN heterostructures, has an influence on the strain of the AlGaN barrier layer,[12,13] the relative permittivity is also related to the device processing, while this calculation ($\varepsilon = 9.5 - 0.5x$) does not include the influence of the device processing on it. Corresponding to Ref.[2], the relative permittivity calculated using Eq.(8) depends on the measured capacitance of Schottky contacts on strained AlGaN/GaN heterostructures, and the capacitance measurement is performed after ohmic contacts and Schottky contacts on strained AlGaN/GaN heterostructures are fabricated. Hence, the influence of the device processing on the relative permittivity is included in its calculation (Eq.(8)). Moreover, the values of the relative permittivity calculated by Eq.(1) are also not the same as those calculated by Eq.(8). This is because the general capacitance value of C is related to the capacitance values of both C_1 and C_2; the capacitance value of C_2 is usually much larger than that of C_1, and so the general capacitance value of C is mainly determined by the capacitance value of C_1 (Eq.(1)). As the reverse

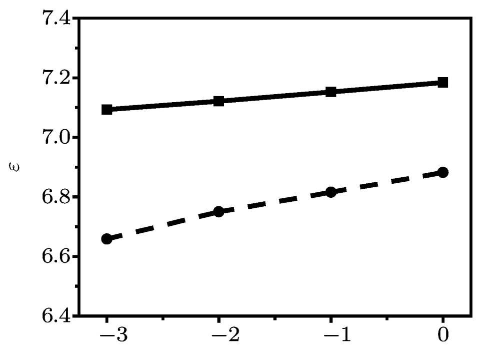

Fig.4. The calculated relative permittivity of the AlGaN barrier layer at different biases. (The solid line and dashed line are calculated with Eq.(1) and Eq.(8) in this paper, respectively).

bias increases, the capacitance value of C_2 becomes small, and the difference of the relative permittivity calculated with the different methods (corresponding to Eq.(1) and Eq.(8)) in Fig.4 increases. As a result, the value of the relative permittivity calculated using Eq.(1) is more precise compared to those in Refs.[1] and [2].

In addition, it is also shown that the value of the relative permittivity of the AlGaN barrier layer decreases with increasing reverse bias. As the reverse bias increases from 0 V to –3 V, the value of the relative permittivity decreases from 7.184 to 7.093. This can be attributed to the increase of the tensile strain in the AlGaN barrier layer with increasing the reverse bias.[14] Therefore, the reverse biasing of the Schottky contact on the strained AlGaN/GaN heterostructure has an influence on the value of the relative permittivity of the AlGaN barrier layer, and as the reverse bias increases, the value of the relative permittivity decreases.

4. Summary

In summary, Ni Schottky contacts were deposited on strained AlGaN/GaN heterostructures. Combining self-consistent solutions of Schrödinger's and Poisson's equations with the measured C–V curve and the photocurrent spectrum for the Ni Schottky contact on strained AlGaN/GaN heterostructures, values of the relative permittivity of the AlGaN barrier layer have been precisely calculated. It is found that the calculated values of the relative permittivity of the AlGaN barrier layer are different from those formerly reported. It is also shown that reverse biasing the Schottky contact on the strained AlGaN/GaN heterostructure has an influence on the value of the relative permittivity of the AlGaN barrier layer, and as the reverse bias increases, the value of the relative permittivity decreases.

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