Influence of thermal stress on the characteristic parameters of AlGaN/GaN heterostructure Schottky contacts*

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Ni Schottky contacts on AlGaN/GaN heterostructures have been fabricated. The samples are then thermally treated in a furnace with N_2 ambient at 600 °C for different times (0.5, 4.5, 10.5, 18, 33, 48 and 72 h). Current–voltage (I–V) and capacitance–voltage (C–V) relationships are measured, and Schrödinger's and Poisson's equations are self-consistently solved to obtain the characteristic parameters related to AlGaN/GaN heterostructure Schottky contacts: the two-dimensional electron gas (2DEG) sheet density, the polarization sheet charge density, the 2DEG distribution in the triangle quantum well and the Schottky barrier height for each thermal stressing time. Most of the above parameters reduce with the increase of stressing time, only the parameter of the average distance of the 2DEG from the AlGaN/GaN interface increases with the increase of thermal stressing time. The changes of the characteristic parameters can be divided into two stages. In the first stage the strain in the AlGaN barrier layer is present. In this stage the characteristic parameters change rapidly compared with those in the second stage in which the AlGaN barrier layer is relaxed and no strain is present.

Keywords: AlGaN/GaN heterostructures, thermal stressing, polarization, self-consistently solving Schrödinger's and Poisson's equations

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1. Introduction

AlGaN/GaN heterostructure field-effect transistors (HFETs) have been a subject of intense investigation and are excellent candidates for high-voltage and high-power operations at microwave frequency.[1−3] The thermal stability of Schottky gate contacts on AlGaN/GaN heterojunctions have a significant influence on the device performances of GaN-based HFETs at high temperatures.[4,5] Previous work on Schottky contacts in AlGaN/GaN heterostructures mainly focused on the effects of annealing on electrical properties such as reduction of reverse leakage current or the improvement of the Schottky barrier height and breakdown voltage.[6,7] Little attention has been paid to the effects of annealing on the characteristic parameters of the Schottky contacts on AlGaN/GaN heterostructures, such as the depth of the triangle quantum well at the AlGaN/GaN interface, the two-dimensional electron gas (2DEG) distribution in the triangle quantum well, the Fermi level of the 2DEG and the strain of the AlGaN barrier layer, although these characteristic parameters are directly related to the above electrical properties of Schottky contacts on AlGaN/GaN heterostructures. In addition, the electrical properties of Schottky contacts on AlGaN/GaN heterostructures are usually determined by these device structure characteristics. As a result, in order to improve AlGaN/GaN HFETs performance at high

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temperature, it is necessary to investigate the influence of annealing on the characteristic parameters of Schottky contacts on AlGaN/GaN heterostructures.

In the work reported here, Ni Schottky contacts on AlGaN/GaN heterostructures have been prepared and the samples are then thermally treated in a furnace with N_2 ambient at 600 °C for different times (0.5, 4.5, 10.5, 18, 33, 48 and 72 h). From the measured current–voltage (I–V) curves and the capacitance–voltage (C–V) curves of each sample, the 2DEG sheet carrier density, the Fermi level of the 2DEG electrons and the 2DEG distribution in the triangle quantum well, the triangle quantum well depth, the Schottky barrier height and the polarization sheet charge density of each sample are obtained by self-consistently solving Schrödinger's and Poisson's equations.

2. Experiment

The heterostucture layer employed in this study was epitaxially grown by metal organic chemical vapour deposition (MOCVD) on a (0001) sapphire substrate. The heterostructure layer consisted of a 40-nm AlN nucleation layer, followed by a 3-μm thick undoped GaN layer 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 the device processing, 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. Ni/Au (60 nm/200 nm) circular Schottky contacts with a diameter of 120 μm were then deposited by e-beam evaporation. The separation between the Ohmic contact and the circular Schottky contact was 20 μm. To examine the influence of thermal stressing time on the characteristic parameters of AlGaN/GaN heterostructure Schottky contacts, samples were then thermally treated in a furnace with N_2 ambient at 600 °C for different times (0.5, 4.5, 10.5, 18, 33, 48 and 72 h). The C–V measurements were performed using an Aglient 4284A LCR meter, and a combination of an ac-modulation voltage of amplitude of ±0.1 V at a frequency of 10 kHz with a dc-biased voltage was used between the Schottky and the Ohmic contacts. The I–V measurements were performed using an Agilent 4156 semiconductor parameter analyser.

3. Calculation and analyses

Figures 1 and 2 respectively show the measured I–V curves and C–V curves at room temperature for the Ni Schottky contacts on $Al_{0.3}Ga_{0.7}N$/GaN heterostructures for the different thermal stressing times. The 2DEG sheet carrier density n_{2D} under Schottky contact metal at zero gate bias can be obtained by the C–V curve integration[6,8]

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

where q is the electron charge, 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,[8] S is the Ni Schottky contact area. The calculated results are shown in Fig. 3, as will be discussed in more detail below after the discussion of the determination of the parameters used in this study.

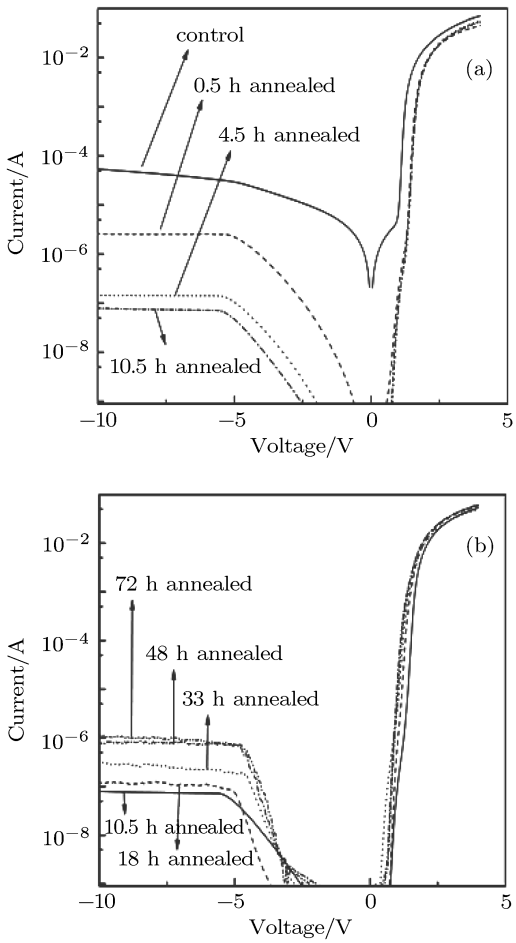


Fig. 1. Measured I–V characteristics of Ni Schottky contacts without (marked with control) and with annealing at 600 °C for different times (0.5, 4.5, 10.5, 18, 33, 48 and 72 h).

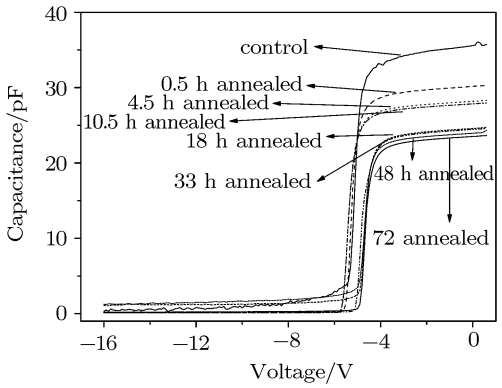


Fig. 2. Measured C–V characteristics of the Ni Schottky contact without (marked with control) and with annealing for different thermal stressing times at 600 °C on $Al_{0.3}Ga_{0.7}N$/GaN heterostructures at room temperature.

The band gap of $Al_xGa_{1-x}N$ at room temperature, used to self-consistently solve Schrödinger's and Poisson's equations, is given by[9]

$$E_g(x) = 6.13x + 3.42(1-x) - x(1-x)\ \text{(eV)}. \quad (2)$$

The conduction-band offset is[10]

$$\Delta E_c = 0.7[E_g(x) - E_g(0)]. \quad (3)$$

In the calculation of Eqs. (2) and (3), the Al content is taken to be 0.3 at room temperature, which results in $\Delta E_C = 0.42$ eV.

Here, E_F is defined as the Fermi level in the AlGaN/GaN heterostructure with respect to the GaN conduction-band-edge energy. The value of the triangle quantum well depth (V_{2DEG}) at the AlGaN/GaN interface is defined as the energy at 41.5 nm along the orientation from the AlGaN surface to the GaN layer with respect to the GaN conduction-band-edge energy. Based on the forward I–V curves, the calculated values of ΔE_C, 2DEG sheet carrier density, Schottky barrier height (ϕ_B), Fermi level (E_F), triangle quantum well depth (V_{2DEG}) and the distribution of the 2DEG in the triangle quantum well for each sample can be calculated by self-consistently solving Schrödinger's and Poisson's equations.[11,12] The average distance (d_{2D}) of the 2DEG from the AlGaN/GaN interface can also be calculated by

$$d_{2D} = \frac{\int n(z) \cdot z \mathrm{d}z}{\int n(z) \mathrm{d}z}, \quad (4)$$

where the z is the orientation to the GaN layer from the AlGaN/GaN interface, $n(z)$ is the concentration distribution of the 2DEG electrons in the triangle quantum well in the z direction and $n(z)$ is obtained by self-consistently solving Schrödinger's and Poisson's equations.[11] The calculated results of each sample are shown in Table 1.

Table 1. Summary of the calculated values for the Schottky barrier height (ϕ_B), Fermi level (E_F), triangle quantum well depth (V_{2DEG}) and average distance (d_{2D}) of each sample.

	ϕ_B/eV	E_F/eV	V_{2DEG}/eV	d_{2D}/nm
control	1.34	0.325	0.391	2.146
0.5 h	1.39	0.287	0.347	2.347
4.5 h	1.46	0.278	0.337	2.400
10.5 h	1.46	0.276	0.335	2.412
18 h	1.46	0.234	0.290	2.697
33 h	1.43	0.231	0.286	2.724
48 h	1.41	0.227	0.283	2.751
72 h	1.41	0.223	0.279	2.782

Using the measured C–V characteristics, the value of the relative permittivity of the AlGaN barrier layer (ε_{AlGaN}) can be calculated by[13]

$$\varepsilon_{AlGaN} = \frac{Cd}{\varepsilon_0 S}, \quad (5)$$

where ε_0 is the vacuum permittivity, and d is the thickness of the AlGaN barrier layer.

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

$$\frac{q(\sigma - n_{2D})}{(E_F + \phi_B - \Delta E_C)} = \frac{\varepsilon_{AlGaN}\varepsilon_0}{d}, \quad (6)$$

in which E_F and ϕ_B are calculated and obtained by self-consistently solving Schrödinger's and Poisson's equations. The calculated polarization sheet charge densities for different thermal stressing times are shown in Fig. 3. The value of the polarization sheet charge density for the control sample (without thermal stressing) was calculated to be 1.26×10^{13} cm^{-2} (Fig. 3). Considering the nonlinearity of the polarization charge as a function of Al composition, Miller *et al.*[15] has calculated the polarization sheet charge density at the $Al_{0.3}Ga_{0.7}N$/GaN interface to be 1.2×10^{13} cm^{-2}, which is very close to our calculated result. Furthermore, taking into account the nonlinear macroscopic polarization in AlGaN/GaN heterostructures, the spontaneous polarization for the $Al_xGa_{1-x}N$ layer, in C/m^2, can be expressed as[16]

$$P^{sp}_{Al_xGa_{1-x}N} = -0.090x - 0.034(1-x) + 0.019x(1-x). \quad (7)$$

The spontaneous polarization sheet charge density in AlGaN/GaN heterostructures can be calculated by

$$\sigma(p_{\rm sp}) = |p^{\rm sp}_{{\rm Al}_x{\rm Ga}_{1-x}{\rm N}} - p^{\rm sp}_{\rm GaN}|/q. \quad (8)$$

Using Eqs. (7) and (8), and taking the Al fraction to be 0.3, the spontaneous polarization sheet charge density of the AlGaN/GaN heterostructure was calculated to be 8.00×10^{12} cm^{-2}. As one can see from Fig. 3, when the thermal stressing time is more than 18 h, the polarization sheet charge density and the 2DEG electron density become approximately constant and the polarization sheet charge density corresponding to the thermal stressing time of 18 h was calculated to be 7.89×10^{12} cm^{-2} (Fig. 3). This calculated value is almost the same as the result calculated by Eqs. (7) and (8), indicating that when the thermal stressing time is increased to 18 h, the AlGaN barrier layer totally relaxes and only spontaneous polarization remains in AlGaN/GaN heterostructures.

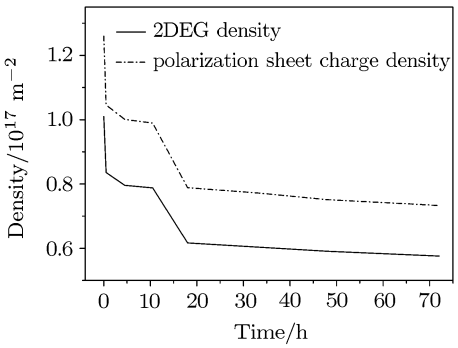


Fig. 3. Calculated 2DEG sheet carrier density and polarization sheet charge density of the Ni Schottky contact without and with annealing for different thermal stressing times at 600 °C on $Al_{0.3}Ga_{0.7}N$/GaN heterostructures at room temperature.

From Table 1 and Fig. 4, one can see that as the thermal stressing time increases the Fermi level goes down, the triangle quantum well depth ($V_{\rm 2DEG}$) decreases and the average distance ($d_{\rm 2D}$) of 2DEG from the AlGaN/GaN interface increases. This is because the quantum confinement effects of the 2DEG electrons are reduced with thermal stressing time increasing. In general, the Schottky barrier height increases or remains unchanged with thermal stressing time increasing, but when the thermal stressing time is more than 18 h, the AlGaN barrier layer totally relaxes and the Schottky barrier height slightly decreases with thermal stressing time increasing until at least 72 h (the longest time studied in this report). The Schottky barrier heights for different thermal stressing times (Table 1) are basically consistent with the reverse saturation currents, i.e., the higher barrier height corresponds to the lower reverse saturation current. The changes for all the above characteristic parameters, which include the 2DEG sheet carrier density and the polarization sheet charge density, are divided into two stages for the different thermal stressing times. In the first stage the strain is present in the AlGaN barrier layer and reduces as a function of stressing time. In the second stage the AlGaN barrier layer has relaxed and therefore no strain is present. The parameters discussed here have a greater change in the first stage.

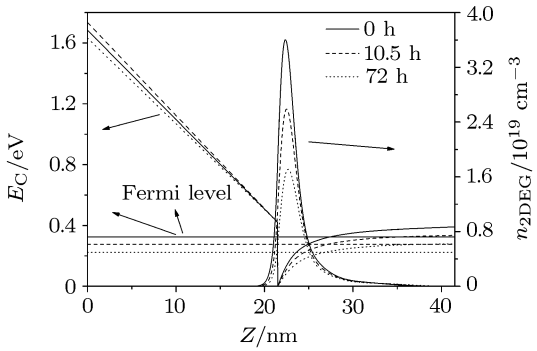


Fig. 4. Conductive bands and the distributions of the 2DEG electrons of the control and those annealed at 600 °C for 10.5 h and 72 h.

4. Conclusions

Ni Schottky contacts on AlGaN/GaN heterostructures have been fabricatedand the samples thermally treated in a furnace with N_2 ambient at 600 °C for different times (0.5, 4.5, 10.5, 18, 33, 48 and 72 h). With the measured I–V and C–V curves and by self-consistently solving Schrödinger's and Poisson's equations, it is found that the characteristic parameters related to AlGaN/GaN heterostructure Schottky contacts such as 2DEG sheet density, polarization sheet charge density, triangle quantum well depth, 2DEG distribution in the triangle quantum well and Schottky barrier height change with the thermal stressing time increasing until the AlGaN barrier totally relaxes (at 18 h in the current study), and then only change slowly with thermal stressing time increasing.

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