Influence of thermal stress on the relative permittivity of the AlGaN barrier layer in an AlGaN/GaN heterostructure Schottky contacts*

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Ni Schottky contacts on AlGaN/GaN heterostructures were fabricated. Some samples were thermally treated in a furnace with N_2 ambience at 600 °C for different times (0.5 h, 4.5 h, 10.5 h, 18 h, 33 h, 48 h, and 72 h), the others were thermally treated for 0.5 h at different temperatures (500 °C, 600 °C, 700 °C, and 800 °C). With the measured current–voltage (I–V) and capacitance–voltage (C–V) curves and by self-consistently solving Schrodinger's and Poisson's equations, we found that the relative permittivity of the AlGaN barrier layer was related to the piezoelectric and the spontaneous polarization of the AlGaN barrier layer. The relative permittivity was in proportion to the strain of the AlGaN barrier layer. The relative permittivity and the strain reduced with the increased thermal stress time until the AlGaN barrier totally relaxed (after 18 h at 600 °C in the current study), and then the relative permittivity was almost a constant with the increased thermal stress time. When the sample was treated at 800 °C for 0.5 h, the relative permittivity was less than the constant due to the huge diffusion of the contact metal atoms. Considering the relation between the relative permittivity of the AlGaN barrier layer and the converse piezoelectric effect, the conclusion can be made that a moderate thermal stress can restrain the converse piezoelectric effect and can improve the stability of AlGaN/GaN heterostructure devices.

Keywords: AlGaN/GaN heterostructures, relative permittivity of AlGaN barrier layer, converse piezoelectric effect

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1. Introduction

The AlGaN/GaN heterostructure field-effect transistors (HFETs) are excellent in high-voltage and high-power operations at microwave frequency,[1−3] and have been a subject of intense investigation. The relative permittivity of the AlGaN barrier layer in the strained AlGaN/GaN heterostructures is a very important parameter of the AlGaN/GaN HFETs, since it is directly related to the polarization sheet charge density of the strained AlGaN/GaN heterostructures.[4] It is also vitally important while self-consistently solving Schrodinger's and Poisson's equations to investigate the characteristic parameters related to AlGaN/GaN heterostructure Schottky contacts, such as the two-dimensional electron gas (2DEG) distribution in the triangle quantum well and the Schottky barrier height.[5,6] Moreover, the converse piezoelectric effect in the AlGaN/GaN HFETs is proportional to the relative permittivity of the AlGaN barrier layer. The electrical properties of the Schottky contacts on the AlGaN/GaN heterostructures can be improved by moderate annealing,[7] but little attention has been paid to the effect of the thermal stress on the relative permittivity, and the previous work on the relative permittivity of the AlGaN barrier layer mainly focused on its accurate calculation.[8] In order to improve the performance of AlGaN/GaN heterostructure devices, it is necessary to investigate the

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influence of the annealing on the relative permittivity of the AlGaN barrier layer.

In this work, Ni Schottky contacts on AlGaN/GaN heterostructures have been prepared. Some samples were then thermally treated in a furnace with N_2 ambience at 600 °C for different times (0.5 h, 4.5 h, 10.5 h, 18 h, 33 h, 48 h, and 72 h), the others were thermally treated for 0.5 h at different temperatures (500 °C, 600 °C, 700 °C, and 800 °C). Based on the measured current–voltage (I–V) and capacitance–voltage (C–V) curves, the relative permittivity of the AlGaN barrier layer and the polarization sheet charge density of each sample were calculated by self-consistently solving Schrodinger's and Poisson's equations. Combining with our previous result, we analysed the influence of different thermal stresses on the relative permittivity of the AlGaN barrier layer.

2. Experiment

The heterostructure layer employed in this study was epitaxially grown via 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 undoped GaN layer and a 21.5-nm thick undoped $Al_{0.3}Ga_{0.7}N$ barrier layer. The Hall measurements indicated 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, the Ohmic contacts of Ti/Al/Mo/Au were fabricated by using the e-beam evaporation and the lift-off technique. 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 using e-beam evaporation. The separation between the Ohmic contact and the circular Schottky contact was 20 μm. To investigate the influence of thermal stress on the relative permittivity of the AlGaN barrier layer ($\varepsilon_{\rm AlGaN}$), some samples were thermally treated in a furnace with N_2 ambience at 600 °C for different times (0.5 h, 4.5 h, 10.5 h, 18 h, 33 h, 48 h, and 72 h), the others were thermally treated in a furnace with N_2 ambience for 0.5 h at different temperatures (500 °C, 600 °C, 700 °C, and 800 °C). The C–V measurements were performed at room temperature by using an Aglient 4284A LCR meter at 10 kHz. The I–V measurements were performed by using an Agilent 4156 semiconductor parameter analyser.

3. Calculation and analyses

Figures 1(a), 1(b), and 2(a) show the measured I–V and C–V curves at room temperature for the Ni Schottky contacts on the $Al_{0.3}Ga_{0.7}N$/GaN heterostructures annealed at 600 °C with different thermal stress times (0.5 h, 4.5 h, 10.5 h, 18 h, 33 h, 48 h, and 72 h). Figures 1(c) and 2(b) show the measured I–V and C–V curves at room temperature for the Ni

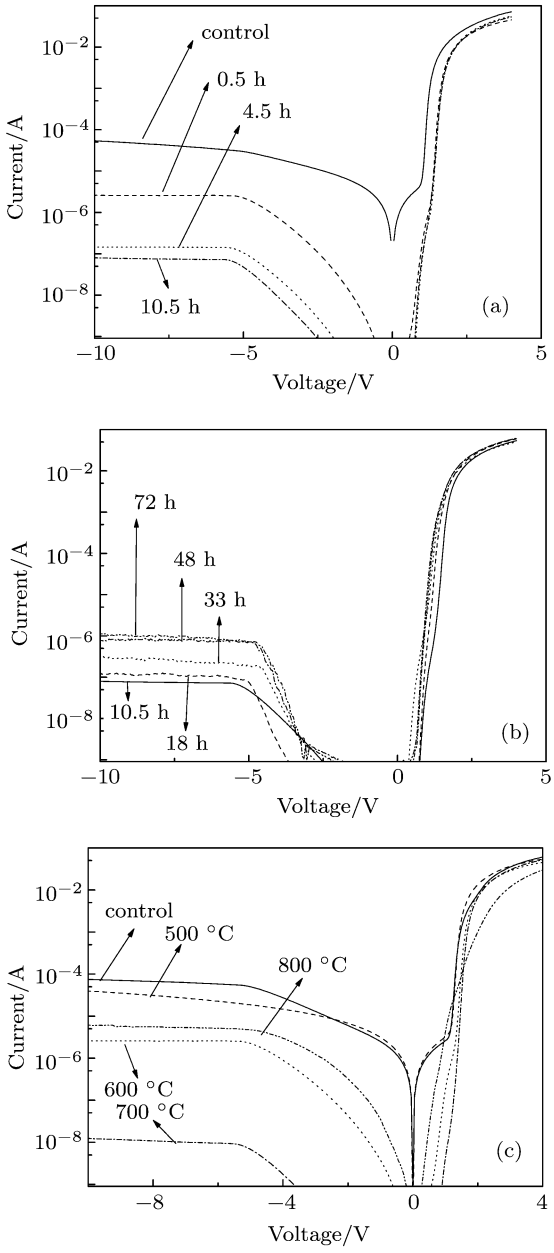


Fig. 1. (a) and (b) Measured I–V characteristics of Ni Schottky contacts without (marked with control) and with annealing at 600 °C for different times (0.5 h, 4.5 h, 10.5 h, 18 h, 33 h, 48 h, and 72 h). (c) Measured I–V characteristics of Ni Schottky contacts without (marked with control) and with annealing for 0.5 h at different temperatures (500 °C, 600 °C, 700 °C, and 800 °C).

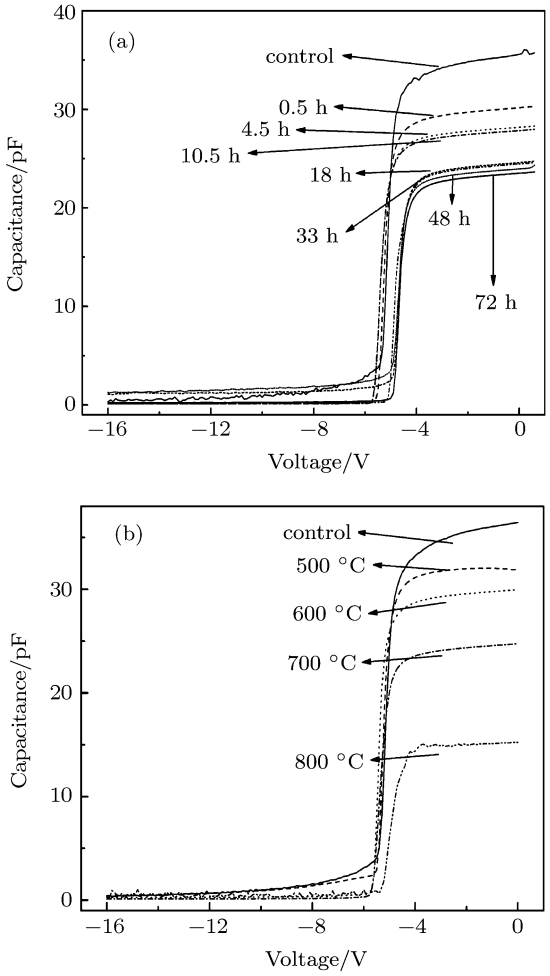


Fig. 2. Measured C–V characteristics of Ni Schottky contact on $Al_{0.3}Ga_{0.7}N$/GaN heterostructures at room temperature (a) without (marked with control) and with annealing for different thermal stress times at 600 °C and (b) without (marked with control) and with annealing for 0.5 h at different temperatures (500 °C, 600 °C, 700 °C, and 800 °C).

Schottky contacts annealed for 0.5 h at different temperatures (500 °C, 600 °C, 700 °C, 800 °C). Using the measured C–V characteristics, we can calculate the value of $\varepsilon_{\mathrm{AlGaN}}$ by[9]

$$\varepsilon_{\mathrm{AlGaN}} = \frac{Cd}{\varepsilon_0 S}, \tag{1}$$

where ε_0 is the vacuum permittivity, d is the thickness of the AlGaN barrier layer, C is the measured capacitance between the Ohmic contact and the Ni Schottky contact, and S is the Ni Schottky contact area. The calculated results for the relative permittivity with different thermal stresses are shown in Figs. 3(a) and 3(b).

We can see from Fig. 3(a) that the value of $\varepsilon_{\mathrm{AlGaN}}$ reduces as the thermal stress time increases, and the reduction is from 7.64 (0 h thermal stress) to 5.05 (72 h thermal stress). However, when the thermal stress time is more than 18 h, the value of $\varepsilon_{\mathrm{AlGaN}}$ becomes approximately a constant. From Fig. 3(b), it is found that the value of $\varepsilon_{\mathrm{AlGaN}}$ reduces from 7.64 (0 h thermal stress) to 3.27 (800 °C for 0.5 h). In order to explain the change in the relative permittivity with different thermal stresses, the polarization sheet charge density of the strained AlGaN/GaN heterostructures were calculated by self-consistently solving Schrodinger's and Poisson's equations. The details of the calculation were shown in our previous report,[10] and the result is shown in Figs. 3(a) and 3(b).

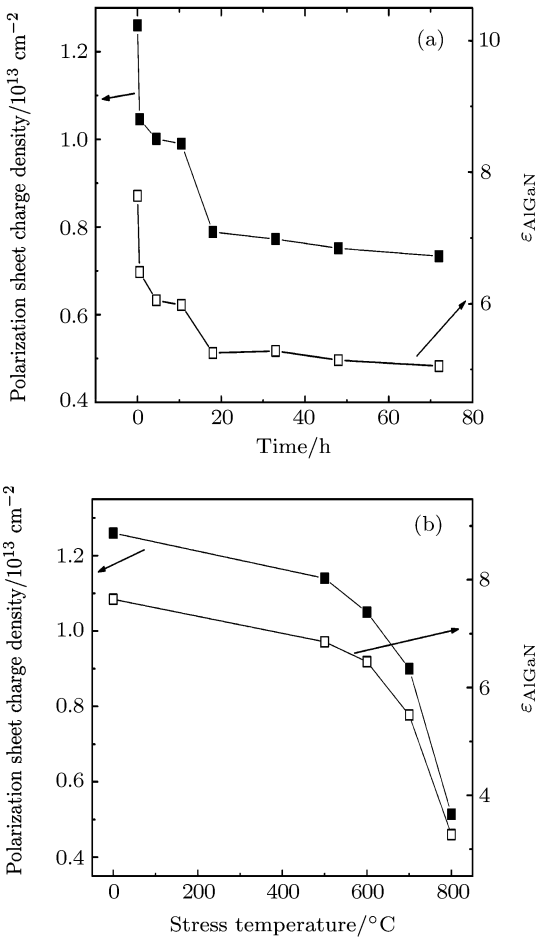


Fig. 3. Calculated room temperature polarization sheet charge density and relative permittivity of Ni Schottky contact on $Al_{0.3}Ga_{0.7}N$/GaN heterostructures (a) without and with annealing for different thermal stress times at 600 °C and (b) with annealing for 0.5 h at different temperatures (500 °C, 600 °C, 700 °C, and 800 °C).

For the samples with different thermal stress time, we previously reported that the changes of the polarization of the AlGaN barrier layer were divided into two stages with different thermal stress times. In the first stage (0 h–18 h), the strain is present in the AlGaN barrier layer and is reduced as a function of the stress time. In the second stage (more than

18 h), the AlGaN barrier layer has relaxed, and therefore no strain is present. Once the thermal time is more than 18 h, there exists only the spontaneous polarization.[10] The spontaneous polarization sheet charge density for the $Al_{0.3}Ga_{0.7}N$/GaN heterostructures is calculated to be 8.00×10^{12} cm^{-2}.[10] As shown in Fig. 3(b), the polarization sheet charge density is larger than 8.00×10^{12} cm^{-2} when the thermal stress temperature is less than 700 °C, and is smaller than 8.00×10^{12} cm^{-2} once the temperature reaches 800 °C. It can be concluded that the thermal stress just affects the strain of the AlGaN barrier layer as a result of the diffusion of the contact metal atoms when the thermal stress temperature is less than 700 °C. Once the temperature reaches 800 °C, the thermal stress changes both the spontaneous and the piezoelectric polarization due to the huge diffusion of the contact metal atoms.

As can be seen from Figs. 3 (a) and 3(b), the changes of the relative permittivity are the same as that of the polarization with different thermal stresses. The conclusion can also be drawn that the relative permittivity of the AlGaN barrier layer is related to the piezoelectric and the spontaneous polarization of the AlGaN barrier layer. The relative permittivity is proportional to the strain of the AlGaN barrier layer. Once the biaxial tensile strain in the AlGaN barrier layer reduces with the thermal stress, the relative permittivity decreases. When the AlGaN barrier layer totally relaxes, the relative permittivity of the AlGaN barrier layer is almost a constant even with the further increasing thermal stress time. However, when the sample is treated at 800 °C for 0.5 h, the spontaneous polarization decreases due to the huge diffusion of the contact metal atoms, and the relative permittivity also decreases to 3.27.

Sarua *et al.*[11] found that the converse piezoelectric effect is going against the stability of the AlGaN/GaN heterostructure devices, since the electric fields generate the strain/stress. Here it is found that the thermal stress can reduce the relative permittivity and the strain of the AlGaN barrier layer, and can further decrease the piezoelectric polarization of the AlGaN barrier layer. Moreover, the value of the relative permittivity is reduced from 7.64 (0 h thermal stressing) to 5.25 (18 h thermal stress at 600 °C) or to 3.27 (800 °C for 0.5 h), and the variation of the relative permittivity is relatively large. Thus, a moderate thermal stress can reduce or restrain the converse piezoelectric effect and can improve the stability of the AlGaN/GaN heterostructure devices. We can see from Figs. 1(a) and 1(b) that the reverse saturation current of the Schottky contacts on the AlGaN/GaN heterostructures decreases with increasing thermal stress time when the time is less than 10.5 h, and increases once the thermal stress time is more than 10.5 h. As shown in Fig. 1(c), the reverse saturation current decreases with increasing thermal temperature when the thermal stress temperature is less than 700 °C, and increases once the temperature reaches 800 °C. So the thermal stress with the appropriate stress time and the appropriate stress temperature can not only reduce the reverse saturation current, but also reduce the relative permittivity of the AlGaN barrier layer, and thus can improve the performance of the AlGaN/GaN heterostructure devices.

4. Conclusion

Ni Schottky contacts on AlGaN/GaN heterostructures have been fabricated. Some samples were thermally treated in a furnace with N_2 ambience at 600 °C for different times (0.5 h, 4.5 h, 10.5 h, 18 h, 33 h, 48 h, and 72 h), the others were thermally treated for 0.5 h at different temperatures (500 °C, 600 °C, 700 °C, and 800 °C). With the measured current–voltage (I–V) and capacitance–voltage (C–V) curves and by self-consistently solving Schrodinger's and Poisson's equations, we found that the relative permittivity of the AlGaN barrier layer was related to the piezoelectric and the spontaneous polarization of the AlGaN barrier layer. The relative permittivity was proportional to the strain of the AlGaN barrier layer. The relative permittivity and the strain reduced with increased thermal stress time at 600 °C until the AlGaN barrier totally relaxed (after 18 h in the current study), and then the relative permittivity was almost a constant with the increased thermal stress time. When the sample was treated at 800 °C for 0.5 h, the relative permittivity was less than the constant due to the huge diffusion of the contact metal atoms. As a result, a moderate thermal stress can restrain the converse piezoelectric effect and can improve the stability of the AlGaN/GaN heterostructure devices.

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