Thermal Stability of Strained AlGaN/GaN Heterostructures

ZHANG Min(张敏), XIAO Hong-Di(肖洪地), LIN Zhao-Jun(林兆军)*

School of Physics and Microelectronics, Shandong University, Jinan 250100

(Received 14 December 2005)

The thermal stability of strained AlGaN/GaN heterostructures is characterized by comparing unannealed and 700°C 30-min annealed Ni Schottky contacts prepared on strained AlGaN/GaN heterostructures. Using photoemission, capacitance–voltage measurements, and the self-consistent solution of Schrodinger's and Poisson's equations, it is found that after 700°C 30-min thermal annealing the Schottky barrier height of Ni Schottky contacts on strained AlGaN/GaN heterostructures is increased, and the sheet density of polarization charges and the sheet density of two-dimensional electron gas (2DEG) electrons for the strained AlGaN/GaN heterostructures are reduced. These results are closely related to the performance of AlGaN/GaN HFETs at high temperature.

PACS: 73. 40. Kp, 85. 30. −Z, 72. 80. Ey

AlGaN/GaN heterostructure field effect transistors (HFET) have been a subject of intense investigation owing to the potentials for high power, high frequency and high temperature applications.[1,2] It has been shown that the piezoelectric and spontaneous polarization can exert a substantial influence on the concentration and distribution of free carriers in strained AlGaN/GaN HFETs.[3,4] With the high temperature application of AlGaN/GaN HFETs, the thermal stability of the strained AlGaN/GaN heterostructures, such as 2DEG sheet density, polarization charge sheet density and Schottky barrier height, is very important. However, so far there have been only a few reports on the thermal stability of strained AlGaN/GaN heterostructures.[5−7] In this work, Ni Schottky contacts are prepared on strained AlGaN/GaN heterostructures, and are thermally annealed at 700°C for 30 min. Photoemission and capacitance-voltage (C–V) measurements are performed for the unannealed and thermal annealed Ni Schottky contacts, respectively. Schrodinger's equation and Poisson's equation are solved self-consistently for the strained AlGaN/GaN heterostructures. Combining the measured results with self-consistently solved results, we investigate the thermal stability of strained AlGaN/GaN heterostructures.

The heterostructure layer employed in this study was epitaxially grown by metalorganic chemical vapour deposition (MOCVD) on a (0001) sapphire substrate. It consists of a 40-nm AlN nucleation layer, followed by a 3-μm undoped GaN and a 21.5-nm-thick undoped $Al_{0.3}Ga_{0.7}N$ barrier layer. Hall measurement indicates a sheet carrier density of around $1.36\times 10^{13}\,cm^{-2}$ and an electron mobility of $1200\,cm^2/Vs$ at room temperature. For the device processing, ohmic contacts of Ti/Al/Mo/Au were deposited 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 circular Schottky contact was 20 μm. The samples were thermally annealed in a furnace with N_2 ambient at 700°C for 30 minutes. The C–V measurements were performed by using an Aglient 4284A LCR meter at a frequency of 10 kHz. The photoemission measurement was performed with a halogen lamp as a light source, a monochromator (ISA, model HR-320) and a lock-in amplifier (EG&G, model 5209) was used for the photocurrent measurement.

Schrodinger's equation (1) and Poisson's equation (2) are solved self-consistently:

$$\Big[-\frac{\hbar^2 d^2}{2m^* dz^2}+U(z)\Big]\psi_L(z)=E_L\psi_L(z), \qquad (1)$$

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; m^* is the effective electron mass in GaN; E_L and ψ_L are the eigenenergy and wave function of electrons, respectively. Here $U(z)$ is the potential energy of electrons and is the same as the conduction band edge of AlGaN/GaN heterostructures;

$$\frac{d}{dz}\Big(\varepsilon\frac{d}{dz}\Big)V(z)=qn(z), \qquad (2)$$

where $V(z)$ is the electron electrostatic potential, $n(z)$ is the electron concentration at the point z, and q is the electron charge. Since the AlGaN and GaN layers are undoped, the impact of acceptor, donor and hole charges is not taken into account. Here ε is the dielectric constant of GaN or AlGaN, depending on which

* Email: linzj@sdu.edu.cn

©2006 Chinese Physical Society and IOP Publishing Ltd

region is being solved. We have

$$n(z) = \frac{m^* kT}{\pi\hbar^2} \sum_L \left[|\psi_L(z)|^2 \ln\left(1 + \exp\frac{E_F - E_L}{kT}\right)\right], \tag{3}$$

in which E_F is the Fermi energy, k is Boltzmann's constant, T is the temperature, the summation with respect to L is over the electron eigenstates and the ground state, the first excited state and the second excited state are included in the calculation. Equation (1) is solved by using trial $U(z)$, with solved , E_L and assumed E_F, the $n(z)$ is calculated by Eq. (3). We can put $n(z)$ into Eq. (2) to obtain a new $U(z)(-qV(z) = U(z))$. Substituting new $U(z)$ into Eq. (1), we can operate iteratively the above processes until the difference between the present $U(z)$ value and the former $U(z)$ value is less than a certain value. In addition, Eq. (4) must also be followed in the self-consistent calculation,

$$\varepsilon_0\varepsilon_{\mathrm{AlGaN}}E_1 + q\sigma = \varepsilon_0\varepsilon_{\mathrm{GaN}}E_2, \tag{4}$$

where σ is the sheet density of polarization charge, ε_0 is the vacuum dielectric constant, $\varepsilon_{\mathrm{AlGaN}}$ is the relative dielectric constant of the AlGaN barrier layer, $\varepsilon_{\mathrm{GaN}}$ is the relative dielectric constant of GaN, E_1 is the electric field value of the AlGaN barrier layer at the AlGaN/GaN heterostructure interface, and E_2 is the electric field value of GaN layer at the heterostructure interface. The total length of the self-consistent calculation is 415 Å and includes all the uppermost epilayers and 200 Å of the interior GaN layer.

Figure 1 shows photocurrent spectra of Ni Schottky contacts unannealed and annealed at 700°C for 30 min. According to Fowler's theory,[8] the relationship between the photocurrent per photon, R, and the incident photon energy $h\nu$ is given by[8−10]

$$R \sim (h\nu - q\Phi_B)^2, \tag{5}$$

where $q\Phi_B$ is the Schottky barrier height. This relation is valid when $h\nu - q\Phi_B > 3kT$.[10] Therefore, the Schottky barrier can be obtained from the straight line relationship of the square root of the photocurrent per photon versus the incident photon energy. With photoemission measurements, the Schottky barrier heights of unannealed and thermally annealed Ni Schottky contacts are 1.47 eV and 1.57 eV, respectively. Figure 2 shows the C–V curves of unannealed and thermally annealed Ni Schottky contacts. There is a capacitance platform in the C–V curves. The capacitance platform corresponds to the change of 2DEG charge quantity in the channel under applied ac signal ΔV, and the greater change of 2DEG charge quantity in the channel results in a higher capacitance value. Moreover, the 2DEG charge quantity can be obtained by the C–V curve integration,[11,12] and the 2DEG sheet density n_s can be calculated by

$$n_s = \int_{-16}^{0} \frac{C}{qS} dV, \tag{6}$$

where C is the capacitance value in the C–V curves, V is the voltage value of the C–V curves, S is the area of the Ni Schottky contacts. The calculated 2DEG sheet densities for unannealed and thermally annealed Ni Schottky contacts are $1.18 \times 10^{13}\,\mathrm{cm}^{-2}$ and $6.98 \times 10^{12}\,\mathrm{cm}^{-2}$, respectively. Based on the above data, self-consistent solutions of Schrodinger's and Poisson's equations are performed. The parameters used in the self-consistent solution for unannealed and thermally annealed Ni Schottky contacts are listed in Table 1.

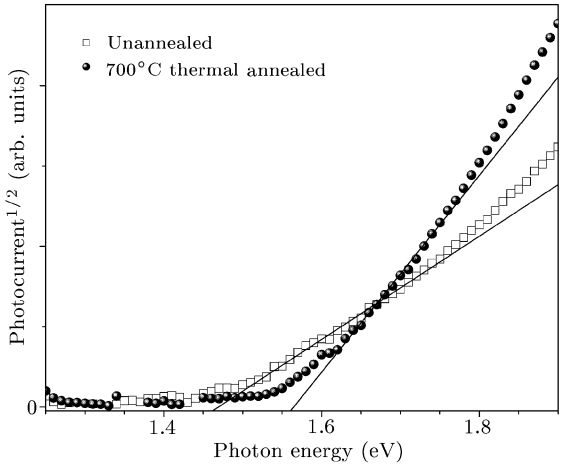


Fig. 1. Photoemission measurement curves for unannealed and 700°C 30-min annealed Ni Schottky contacts.

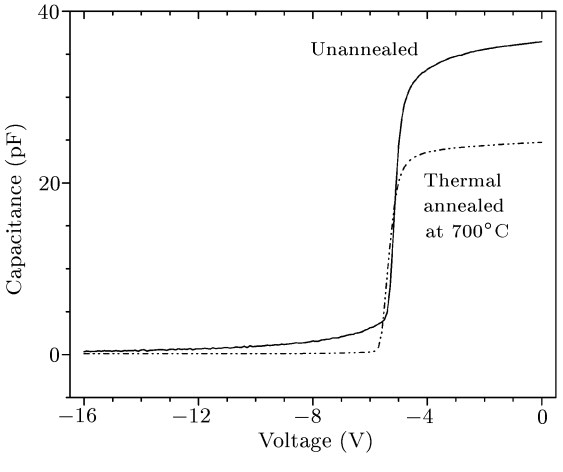


Fig. 2. C–V measurement curves for unannealed and 700°C 30-min annealed Ni Schottky contacts.

In Table 1, ΔE_c is the band offset for $Al_{0.3}Ga_{0.7}N$/GaN heterostructures. The values of ΔE_c, $\varepsilon_{\mathrm{GaN}}$ and $\varepsilon_{\mathrm{AlGaN}}$ are obtained from Ref. [3]. Figure 3 shows the self-consistently solved conduction band edge and the electron concentration for

the AlGaN/GaN heterostructures. It is found that after 700°C 30-min thermal annealing, the triangular quantum well of the AlGaN/GaN heterostructures becomes wider. Moreover, with self-consistent calculation, the sheet density of polarization charges for unannealed and thermally annealed Ni Schottky contacts are obtained and they are $1.56 \times 10^{13}\,\mathrm{cm}^{-2}$ and $1.075 \times 10^{13}\,\mathrm{cm}^{-2}$, respectively. It is shown that after 700°C 30-min thermal annealing, both the electron sheet density of 2DEG and the sheet density of polarization charges for strained AlGaN/GaN heterostructures are reduced, and the Schottky barrier height of Ni Schottky contacts is increased. Since the changes of the above-mentioned parameters are directly related to the performance of thermal annealing in AlGaN/GaN HFETs, the above results are important and valuable for high temperature applications of AlGaN/GaN HFET.

Table 1. The parameters of self-consistent calculation for unannealed and thermally annealed Ni Schottky contacts.

	$q\Phi_B$ (eV)	n_s (cm^{-2})	ΔE_c (eV)	$\varepsilon_{\mathrm{GaN}}$	$\varepsilon_{\mathrm{AlGaN}}$
Unannealed	1.47	1.18×10^{13}	0.42	10.4	10.31
Annealed	1.57	6.98×10^{12}	0.42	10.4	10.31

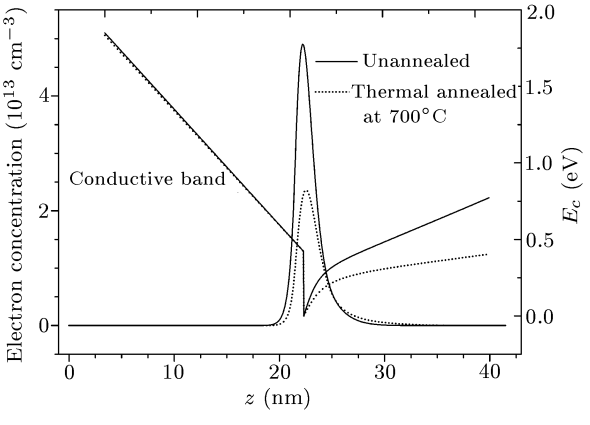


Fig. 3. Conduction band edge and the electron concentration for the unannealed and 700°C 30-min annealed AlGaN/GaN heterostructures.

Ni Schottky contacts were prepared on strained AlGaN/GaN heterostructures and the prepared Ni Schottky contacts were thermally annealed with 700°C 30-min. With photoemission, capacitance-voltage measurements, and self-consistent solving Schrodinger's equation and Poisson's equation, the Schottky barrier height, the sheet electron density of 2DEG and the sheet density of polarization charges for the prepared Ni Schottky contacts on strained AlGaN/GaN heterostructures are obtained. It is shown that after 700°C 30-min thermal annealing, the Schottky barrier height of Ni Schottky contacts on strained AlGaN/GaN heterostructures is increased, and the sheet density of polarization charges and the sheet electron density of 2DEG for the strained AlGaN/GaN heterostructures are reduced.

The authors thank Dr Timothy Corrigan for useful discussions and help in the manuscript preparation.

References

[1] Wu Y F, Kapolnek D, Ibbetson J P et al 2001 *IEEE Trans. Electron. Devices* **48** 586
[2] lu W, Kumar V, Schwindt R et al 2002 *IEEE Trans. Microwave Theor. Tech.* **50** 2499
[3] Ambacher O, Foutz B, Smart J et al 2000 *J. Appl. Phys.* **87** 334
[4] Wen b, Jiang R L, Zhou J J et al 2004 *Chin. Phys. Lett.* **21** 720
[5] Feng Z H, Zhou Y G, Cai S J et al 2004 *Appl. Phys. Lett.* **85** 5248
[6] Lee J, Liu D, Kim H et al 2004 *Appl. Phys. Lett.* **85** 2631
[7] Lin Z,J Kim H, Lee J et al 2004 *Appl. Phys. Lett.* **84** 1585
[8] Fowler R H 1931 *Phys. Rev.* **38** 45
[9] Sze S M 1981 *Physics of Semiconductor Devices* (New York: Wiley) chap 5
[10] Crowell C R, Spitzer W G, Howarth L E et al 1962 *Phys. Rev.* **127** 2006
[11] Lin Z J, Lu W, Lee J et al 2003 *Appl. Phys. Lett.* **82** 4364
[12] Lin Z J, Lu W, Lee J et al 2003 *Electron. Lett.* **39** 1412