Barrier heights of Schottky contacts on strained AlGaN/GaN heterostructures: Determination and effect of metal work functions

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Ir, Ni, and Re Schottky contacts on strained $Al_{0.25}Ga_{0.75}N/GaN$ heterostructures are characterized using capacitance–voltage ($C-V$) and $I-V$ techniques. Based on the measured $C-V$ characteristics, two dimensional electron gas sheet carrier concentrations at the AlGaN/GaN interface and barrier heights of Ir, Ni, and Re Schottky contacts are calculated. The barrier heights of 1.12, 1.27, and 1.68 eV are obtained for Ir, Ni, and Re Schottky contacts, respectively. The results show that the barrier heights of Schottky contacts on strained AlGaN/GaN heterostructures are strongly dependent on the metal work functions. However, contrary to Schottky contacts on bulk AlGaN or GaN, the barrier height on strained AlGaN/GaN heterostructures is lower for a Schottky contact with a higher metal work function. This is attributed to the stronger wave function coupling between electrons in the Schottky metal and surface donor electrons. The $I-V$ characteristics for Ir, Ni, and Re Schottky contacts confirm the results obtained by $C-V$ characteristics. [DOI: 10.1063/1.1584077]

AlGaN/GaN high electron mobility transistors (HEMTs) are excellent candidates for high power applications at microwave frequencies because of the unique material properties.[1,2] It has been shown that piezoelectric and spontaneous polarization exerts a substantial influence on the concentration and distribution of free carriers in strained AlGaN/GaN HEMT heterostructures.[3,4] For an AlGaN/GaN power HEMT, a Schottky gate contact with a large barrier height is always desirable to achieve low gate leakage current, high breakdown voltages, and high turn-on voltages. So far, investigations have been focused on Schottky contacts on bulk AlGaN and GaN,[5] where the piezoelectric polarization effects are not existed. On bulk GaN or AlGaN, the barrier heights are higher for Schottky contacts with higher metal work functions. In addition, barrier heights of Schottky contacts on strained AlGaN/GaN heterostructures cannot be determined by conventional thermionic emission theory because of the existence of strong polarization piezoelectric effect. Therefore, it is important to investigate the polarization effect on characteristics of Schottky contacts on strained AlGaN/GaN heterostructures. In this letter, we report a method to determine barrier heights of Schottky contacts on AlGaN/GaN heterostructures using capacitance–voltage ($C-V$) measurements. The barrier heights of Ir, Ni, and Re Schottky contacts on strained $Al_{0.25}Ga_{0.75}N/GaN$ heterostructures are characterized. The effects of metal work function on Schottky barrier heights are discussed.

The layer used in this study was epitaxially grown by metalorganic chemical vapor deposition on a (0001) sapphire substrate. It consists of a 40 nm AlN nucleation layer, followed by a 3 μm undoped GaN, and a 20-nm-thick undoped $Al_{0.25}Ga_{0.75}N$. Hall measurement indicates a sheet carrier density of 9×10^{12} cm^{-2} and an electron mobility of 1100 $cm^2/V\,s$ at room temperature. For device processing, Ohmic contacts of Ti/Al/Mo/Au were performed by electron (e)-beam evaporation and lift-off. The contacts were then annealed at 900 °C for 30 s in a rapid thermal annealing system. Circular Schottky contacts of Ni/Au (60 nm/300 nm), Ir (150 nm), and Re (200 nm) with a diameter of 120 μm were then deposited by e-beam evaporation in three samples separately. The separation between the Ohmic contact and circular Schottky contact is 40 μm. $C-V$ measurements were performed using an Agilent 4284A LCR meter at a frequency of 10 kHz. $I-V$ measurements were performed using an Agilent 4156C semiconductor parameter analyzer.

The strained $Al_{0.25}Ga_{0.75}N/GaN$ layer structure, the conduction-band energy diagram, the distribution of polarization-induced charge, surface states (σ_{surf}), and free-carrier charge (σ_{2deg}) are shown in Fig. 1. The polarization-

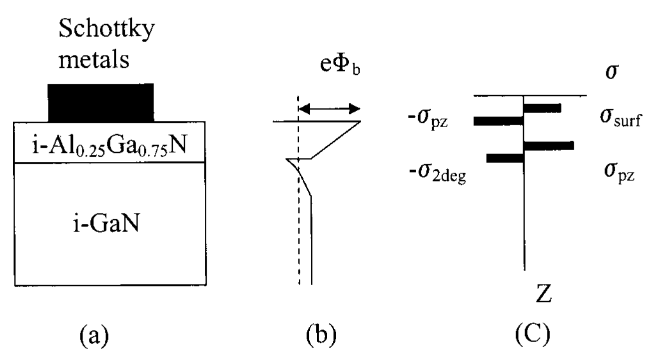

FIG. 1. (a) Schematic diagram of an undoped $Al_{0.25}Ga_{0.75}N/GaN$ HFET structure. (b) Conduction-band energy diagram; the dotted line represents the Fermi level, and $e\Phi_b$ is the Schottky barrier height. (c) Schematic diagram of surface states, polarization-induced and free-carrier charge distribution.

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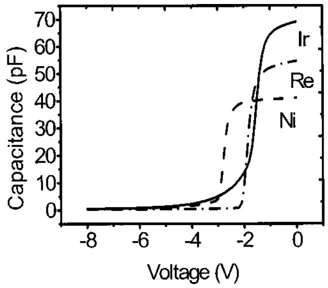

FIG. 2. Capacitance–voltage characteristics of Ir, Ni, and Re Schottky contacts on $Al_{0.25}Ga_{0.75}N$/GaN heterostructure at room temperature.

induced charges σ_{pz} and $-\sigma_{pz}$ are formed at the AlGaN/GaN interface and at the AlGaN surface, respectively, due to the strong polarized electric field in the strained $Al_{0.25}Ga_{0.75}N$ layer. The electrons of $Al_{0.25}Ga_{0.75}N$ surface states flow to $Al_{0.25}Ga_{0.75}N$/GaN interface and a two-dimensional electron gas (2DEG) is formed.[6] The negative charges cancel partially polarization-induced charges and reduce the polarized electric field.[7] Thus, the sheet charge density of 2DEG is strongly related to the Schottky barrier height. Figure 2 shows the $C-V$ characteristics of Ir, Ni, and Re Schottky contacts on strained $Al_{0.25}Ga_{0.75}N$/GaN heterostructure at room temperature. In Fig. 2, for different metal Schottky contacts, the values of capacitance platforms are different, which correspond to the degree of variation of 2DEG charge quantity in the channel under the applied ac signal (ΔV). Moreover, the 2DEG charge density is decreased when the dc bias is decreased. So, if the change of electron charge in the unintentionally doped buffer is negligible, the 2DEG charge quantity at the AlGaN/GaN interface can be obtained by $C-V$ curve integration. The calculated 2DEG sheet carrier concentrations at the AlGaN/GaN interface for Ir, Ni, and Re Schottky contacts are $6.81\times10^{12}\ \mathrm{cm}^{-2}$, $6.41\times10^{12}\ \mathrm{cm}^{-2}$, and $5.41\times10^{12}\ \mathrm{cm}^{-2}$, respectively. For a nominally undoped HEMT structure with a Schottky gate contact, the 2DEG sheet carrier concentration at the AlGaN/GaN interface is given by[7]

$$n_s(x) = \sigma(x)/e - [\epsilon_0\epsilon(x)/de^2][e\Phi_b(x) + E_F(x) - \Delta E_c(x)], \tag{1}$$

where x is the Al concentration, σ is the polarization sheet charge density, d is the width of the $Al_xGa_{1-x}N$ barrier layer, $e\Phi_b$ is the Schottky barrier height, E_F is the Fermi level with respect to the GaN conduction-band-edge energy, and ΔE_c is the conduction band offset at the AlGaN/GaN interface, ϵ is the dielectric constant of $Al_xGa_{1-x}N$, ϵ_0 is vacuum dielectric constant, and e is electron charge. The Fermi level $E_F(x)$ is calculated by[8]

$$E_F(x) = E_0(x) + [\pi\hbar^2/m^*(x)]n_s(x), \tag{2}$$

where the ground subband level of the 2DEG, $E_0(x)$, is given by

$$E_0(x) = \left[\frac{9\pi\hbar e^2}{8\epsilon_0\sqrt{8m^*(x)}}\,\frac{n_s(x)}{\epsilon(x)}\right]^{2/3}. \tag{3}$$

Here, the effective electron mass, $m^*(x)\approx 0.22m_e$. The band offset, ΔE_c, is determined by[9,10]

$$\Delta E_c = 0.7[E_g(x) - E_g(0)], \tag{4}$$

where the band gap of AlGaN, $E_g(x)$, is given by[11]

$$E_g(x) = 6.13x + 3.42(1-x) - x(1-x)\ \ (\mathrm{eV}). \tag{5}$$

If x is taken as 0.25 and $\epsilon(x)$ as 10.33,[4] the $\Delta E_c(x)$ is calculated to be 0.343 eV. Applying the sheet carrier concentrations (n_s) obtained from $C-V$ characteristics to Eqs. (3) and (2), the $E_F(x)$ are determined to be 0.27, 0.26, and 0.208 eV, respectively, for $Al_{0.25}Ga_{0.75}N$/GaN heterostructures with Ir, Ni, and Re Schottky contacts. The Schottky barrier heights are obtained by substituting the above values into Eq. (1). The barrier heights are determined to be 1.12, 1.27, and 1.68 eV for Ir, Ni, and Re Schottky contacts, respectively. In this calculation, $\sigma(x)$ is estimated[4] as $9.8\times10^{12}\ \mathrm{cm}^{-2}$, and AlGaN layer thickness d is 20 nm. If one considers that the metal work functions of Ir, Ni, and Re are 5.62, 5.15, and 4.72 eV, respectively,[12] the results indicate that the barrier height is lower for a Schottky contact on strained AlGaN/GaN heterostructure with a higher metal work function, which is contrary to what people have observed on Schottky contacts on bulk $Al_xGa_{1-x}N$ and GaN semiconductors and deserves an explanation. In strained undoped AlGaN/GaN heterostructures, surface donors of AlGaN barrier layer are considered to be the source of 2DEG electrons.[6] The energies of electrons in metal with a lower work function are higher. These electrons with higher energies have larger moving spaces. As a result, their electron wave functions have more overlapping with that of $Al_xGa_{1-x}N$ surface donor electrons, which results in stronger coupling between electrons in the metals and AlGaN surface donor electrons. The stronger coupling has the larger influence on the characteristics of AlGaN surface states, such as surface state density and surface state energy levels, which affect directly on 2DEG sheet carrier concentration. This is shown by the differences between our calculated 2DEG sheet carrier concentrations with different Schottky metal contacts (Ir: $6.81\times10^{12}\ \mathrm{cm}^{-2}$, Ni: $6.41\times10^{12}\ \mathrm{cm}^{-2}$, and Re: $5.41\times10^{12}\ \mathrm{cm}^{-2}$) and the sheet carrier concentration ($9.0\times10^{12}\ \mathrm{cm}^{-2}$, with no Schottky metal contacts) determined by Hall measurements. It should be pointed out here that such difference in sheet carrier concentration increases if the metal work function decreases. The negative 2DEG electron charges cancel partially polarization-induced charges. So, at the same polarization sheet charge density, barrier heights of Schottky contacts are higher because of the decrease of 2DEG sheet carrier concentration. Therefore, with the larger influence on AlGaN surface states, the barrier heights are higher for Schottky contacts on strained AlGaN/GaN heterostructures with lower metal work functions.

In another aspect, the 2DEG density is related to the electric field value on the GaN side of the interface between AlGaN barrier layer and GaN buffer layer. A higher 2DEG sheet carrier concentration corresponds to a larger electric field value.[13] Then a higher voltage would be required to pinch off the channel with a larger electric field value at the AlGaN/GaN interface. Figure 3 shows $I-V$ characteristics of Ir, Ni, and Re Schottky contacts at room temperature. As shown in Fig. 3, the saturation current of Re Schottky diode is the smallest, indicating that Re/AlGaN/GaN structure has the lowest 2DEG concentration at the AlGaN/GaN interface.

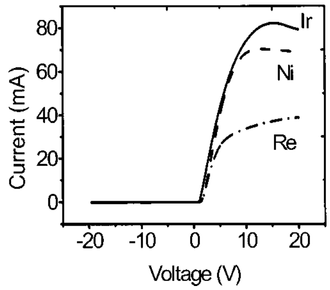

FIG. 3. Current–voltage characteristics of Ir, Ni, and Re Schottky contacts on $Al_{0.25}Ga_{0.75}N/GaN$ heterostructure at room temperature.

This is consistent with the results obtained using $C-V$ techniques. Moreover, a lower 2DEG concentration corresponds to a higher barrier height in the structures studied in this work.

In summary, we have proposed a method to determine the barrier height of a Schottky contact on strained AlGaN/GaN heterostructures based on $C-V$ characteristics. Using this technique, the 2DEG sheet carrier concentrations and barrier heights of Ir, Ni, and Re Schottky contacts on strained $Al_{0.25}Ga_{0.75}N/GaN$ heterostructures are calculated. The results show that the barrier height of a Schottky contact with a lower metal work function is higher on strained AlGaN/GaN heterostructures. This is attributed to the influence of Schottky contact metal on the surface states of AlGaN barrier layer. The measured $I-V$ results for Ir, Ni, and Re Schottky contacts are consistent with our calculated 2DEG sheet carrier concentrations and barrier heights.

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