Simulation of Tunneling Contact Resistivity in Non-polar AlGaIn/GaN Heterostructures

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SUMMARY We have evaluated the tunneling contact resistivity based on numerical calculation of tunneling current density across an AlGaIn barrier layer in non-polar AlGaIn/GaN heterostructures. In order to reduce the tunneling contact resistivity, we have introduced an n^+ -Al_xGa_{1-x}N layer between an n^+ -GaN cap layer and an i -AlGaIn barrier layer. The tunneling contact resistivity has been optimized by varying Al composition and donor concentration in n^+ -Al_xGa_{1-x}N. Simulation results show that the tunneling contact resistivity can be improved by as large as 4 orders of magnitude, compared to the standard AlGaIn/GaN heterostructure.

key words: GaN, HEMT, potential barrier, contact resistance, tunneling current density

1. Introduction

High electron mobility transistors (HEMTs) based on an AlGaIn/GaN heterostructure have attracted significant attention as high-frequency and high-power electronic devices, such as power amplifiers and high-voltage low-loss switching elements [1]. This is due to the high saturation electron velocity and high breakdown field of GaN and related III-nitride semiconductors. However, it is well-known that the parasitic resistance components, such as contact resistance, have an adverse influence on the device performance, such as transconductance, switching efficiency and current gain cutoff frequency [2]–[5]. Furthermore, the contact resistance is known as rather a difficult component to reduce since an AlGaIn barrier layer prevents electrons from transferring from ohmic electrodes to a GaN channel.

Typical conduction band energy diagrams and electron density profiles for polar and non-polar double heterostructures are shown in Fig. 1. In the polar double heterostructure, the potential shape in a GaN channel becomes acute triangular since there are positive and negative polarization charges at the upper and the lower AlGaIn/GaN hetero-interfaces, as shown in Fig. 1(a). The strong triangular potential profile, however, gives rise to some undesirable limitations in the control of two-dimensional electron gas (2DEG) density, such as a reduced maximum 2DEG density and rather a poor control of the threshold voltage in an enhancement-mode operation. On the other hand, the non-polar double heterostructure, as shown in Fig. 1(b), is expected to show a high 2DEG density due to the double

Fig. 1 Conduction band energy diagrams (solid line) and electron density profiles (dotted line) for polar (a) and non-polar (b) double heterostructures.

modulation-doped structure and is suited for a precise control in the threshold voltage because the channel electron density is determined only by doping.

In the non-polar structure, the ohmic contact resistance is primarily limited by electron tunneling transport through the surface AlGaIn barrier layer. However, to the best of our knowledge, no theoretical study has been made on the calculation of tunneling resistivity in non-polar AlGaIn/GaN/AlGaIn double heterostructures.

In this paper, we report simulation results of tunneling current density across an AlGaIn barrier layer and propose an optimum design procedure for non-polar AlGaIn/GaN heterostructures with a reduced contact resistivity.

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2. Simulation Procedure and Device Structure

In this work, for the purpose of analyzing electronic states in AlGaIn/GaN heterojunction interfaces, we have self-consistently solved Schrödinger equation coupled with Poisson equation, expressed as Eqs. (1) and (2), respectively [6],

$$-\frac{\hbar^2}{2} \frac{d}{dz} \frac{1}{m(z)} \frac{dF_i(z)}{dz} + V(z)F_i(z) = E_i F_i(z) \quad (1)$$

$$\frac{d}{dz} \epsilon(z) \frac{d\phi(z)}{dz} = q \left[\sum_{i=1}^m N_i F_i^2(z) + N_A(z) - N_D(z) \right] \quad (2)$$

where F_i is the envelope function for an electron in subband i , $m(z)$ is the position-dependent effective mass, E_i is the energy for i th subband, V is an effective potential, ϕ is the electrostatic potential, N_i is the sheet electron density in i th subband, N_A (N_D) is the acceptor (donor) concentration. This simulator calculates electronic states by dividing the device into segments. The thickness of unit segment was 1 Å. The self-consistent calculation was repeated until the absolute difference between new and previous potential energy values converges to a predetermined value of 1×10^{-6} V. Once the convergence is reached, the tunneling current density was calculated as described below.

Figure 2 shows the conduction band energy diagram used for calculating the tunneling current density across the potential barrier. The broken line denotes the conduction band potential energy at zero bias and the solid line denotes the potential energy under the biasing condition. By assuming Fermi-Dirac distribution, the tunneling current density for an electron with energy E_Z is given by Eq. (3) [7]–[11],

$$J(V, E_Z) = \frac{qm_0^* kT}{2\pi^2 \hbar^3} D(E_Z) \times \ln \left[\frac{1 + \exp\{(E_F - E_Z)/kT\}}{1 + \exp\{(E_F - qV - E_Z)/kT\}} \right] \quad (3)$$

where $D(E_Z)$ is the tunneling probability, V is the applied voltage, E_Z is the electron energy. The tunneling probability was evaluated from the continuity of wave function and its derivative at each boundary.

Total tunneling current density $J(V)$ was calculated by integrating $J(V, E_Z)$ with respect to the electron energy E_Z . From the plot of total tunneling current density $J(V)$ as a

Fig. 2 Conduction band energy diagram used for calculating tunneling current density across potential barrier.

function of the applied voltage V , the tunneling contact resistivity ρ_c for an arbitrary potential barrier is evaluated by $\rho_c = [\Delta J(V)/\Delta V]^{-1}|_{V=0}$.

Figure 3 shows the cross sectional structure of a non-polar AlGaIn/GaN heterostructure studied in this work. The device consists of a non-polar GaN substrate, an i-AlGaIn barrier layer, an i-GaN channel layer, an i-AlGaIn barrier layer, an n^+ -AlGaIn layer and an n^+ -GaN cap layer. In order to reduce the tunneling contact resistivity, we have introduced an n^+ -AlGaIn layer between an n^+ -GaN cap and a barrier layer. The thicknesses for n^+ -GaN, n^+ -AlGaIn and i-AlGaIn layers were 20, 10 and 20 nm, respectively. The donor concentration in an n^+ -GaN layer (N_{d1}) was assumed to be $1 \times 10^{20} \text{ cm}^{-3}$. The lattice temperature and Schottky barrier height were 300 K and 0.8 eV, respectively. To achieve high 2DEG density in the channel, two Si delta-doped layers with $1 \times 10^{13} \text{ cm}^{-2}$ were spaced 2 nm away from the interface between an AlGaIn layer and a GaN channel layer.

Figure 4 shows three components of tunneling contact resistivity under the source electrode. The total contact resistivity $\rho_c (= \rho_{c1} + \rho_{c2} + \rho_{c3})$ was defined as the sum of resistivity components between the source and the GaN channel, where ρ_{c1} , ρ_{c2} and ρ_{c3} are the tunneling contact resistivities across an n^+ -GaN cap, an n^+ -AlGaIn layer and an

Fig. 3 Cross sectional structure of non-polar AlGaIn/GaN heterostructure assumed in our simulation.

Fig. 4 Three components of tunneling contact resistivity under source electrode. Total tunneling contact resistivity was defined as sum of resistivity components between source and GaN channel.

i-AlGaIn barrier layer, respectively. These resistivity components were evaluated by applying a small bias voltage across each potential barrier, in a similar procedure as that described above. In this analysis, we have attempted to minimize the total tunneling contact resistivity by varying the Al composition and the donor concentration in an n^+ -AlGaIn layer.

3. Results and Discussions

Figure 5 shows the conduction band energy diagram for the device structure without an n^+ -AlGaIn layer. The values of tunneling contact resistivity across an n^+ -GaIn cap and an i-AlGaIn barrier layer were 1.7×10^{-7} and $3.6 \times 10^{-2} \Omega\text{cm}^2$, respectively. Because of the extremely thin potential barrier thickness at the semiconductor surface, the resistivity ρ_{c1} is negligibly small, whereas the resistivity ρ_{c3} (in i-AlGaIn) is appreciably high since the i-AlGaIn barrier layer has a long tunneling distance with a large conduction band energy discontinuity of 0.49 eV, as calculated using the energy distribution rule reported by Ambacher et al. [12]. Accordingly, the tunneling contact resistivity across the AlGaIn barrier layer becomes dominant in the total contact resistivity.

Figure 6 shows the conduction band energy diagram for

Fig. 5 Conduction band energy diagram for structure without n^+ -AlGaIn layer.

Fig. 6 Conduction band energy diagram for structure with n^+ -AlGaIn layer. Al composition and donor concentration in n^+ -AlGaIn were 0.1 and $1 \times 10^{19} \text{ cm}^{-3}$, respectively.

a device structure with an n^+ -AlGaIn layer. The Al composition, thickness and donor concentration (N_{d2}) in n^+ -AlGaIn were 0.1, 10 nm and $1 \times 10^{19} \text{ cm}^{-3}$, respectively. It is obvious that the potential energy at P_1 (located at the interface between n^+ -GaIn and n^+ -AlGaIn) is much lower than that at P_2 (located at the interface between n^+ -AlGaIn and i-AlGaIn), indicating that the tunneling contact resistivity ρ_{c3} is dominant in the total contact resistivity at $x = 0.1$. The estimated total tunneling contact resistivity ρ_c is $3.0 \times 10^{-4} \Omega\text{cm}^2$, which is about 2 orders of magnitude lower than that of $3.6 \times 10^{-2} \Omega\text{cm}^2$ obtained for the structure without an n^+ -AlGaIn layer.

Figure 7 shows the conduction band energy diagram for a device structure with an increased Al composition of 0.17. With increasing the Al composition, the potential energy at P_1 increases while that at P_2 decreases. Correspondingly, peak potentials at P_1 and P_2 become almost identical at $x = 0.17$. Since the thickness of i-AlGaIn is twice as large as that of n^+ -AlGaIn, the tunneling contact resistivity in i-AlGaIn becomes dominant ($\rho_{c3} = 6.3 \times 10^{-6} \Omega\text{cm}^2$), resulting in the total tunneling contact resistivity ρ_c of $6.7 \times 10^{-6} \Omega\text{cm}^2$.

Figure 8 shows the conduction band energy diagram for the structure with $x = 0.22$. Note that the potential energy at P_1 continues to increase while that at P_2 continues to decrease with increasing Al composition. Thus at $x =$

Fig. 7 Conduction band energy diagram under source electrode for Al composition in n^+ -AlGaIn layer of 0.17.

Fig. 8 Conduction band energy diagram under source electrode for Al composition in n^+ -AlGaIn layer of 0.22.

Fig. 9 Three peak potential energies as a function of Al composition in n^+ -AlGaIn layer.

Fig. 10 Three tunneling contact resistivities as a function of Al composition in n^+ -AlGaIn layer.

0.22, the potential energy at P_1 becomes higher than that at P_2 by about 0.2 eV. Since the thickness of i -AlGaIn is twice as large as that of n^+ -AlGaIn, the tunneling resistivity ρ_{c2} ($= 9.2 \times 10^{-7} \Omega\text{cm}^2$) becomes almost identical to ρ_{c3} ($= 7.2 \times 10^{-7} \Omega\text{cm}^2$). Accordingly, a minimum total tunneling contact resistivity ρ_c of $1.8 \times 10^{-6} \Omega\text{cm}^2$ is obtained at $x = 0.22$, corresponding to about 4 orders of magnitude improvement in the contact resistivity, compared to the structure without an n^+ -AlGaIn layer.

Figure 9 shows potential energies at P_1 , P_2 and P^* as a function of Al composition in n^+ -AlGaIn, where P^* represents the peak potential position in the i -AlGaIn layer. The donor concentration in n^+ -AlGaIn is $1 \times 10^{19} \text{ cm}^{-3}$. Note that P^* becomes larger than P_2 when the Al composition is larger than 0.2. As the potential energy at P_1 linearly increases while that at P_2 gradually decreases with the increase in Al composition, those two potentials coincide at a cross point of $x = 0.17$, as indicated in Fig. 7.

Figure 10 shows the calculated three tunneling contact resistivities (ρ_{c1} , ρ_{c2} and ρ_{c3}) as a function of Al composition in an n^+ -AlGaIn layer. Since the potential profile in n^+ -GaIn is insensitive to the Al composition in n^+ -AlGaIn, ρ_{c1} exhibited no dependence on the Al composition. Corresponding to the potential energy changes at P_1 and P_2 , ρ_{c2}

Fig. 11 Total tunneling contact resistivity as a function of Al composition in n^+ -AlGaIn layer with different donor concentrations of 5×10^{18} , 1×10^{19} and $3 \times 10^{19} \text{ cm}^{-3}$.

increases while ρ_{c3} decreases with increasing the Al composition. The saturation in ρ_{c3} , observed at an Al composition of more than 0.2, is because the peak potential position in i -AlGaIn changes from P_2 to P^* , as shown in Fig. 9. As a result, the total tunneling contact resistivity ρ_c exhibited a minimum value of $1.8 \times 10^{-6} \Omega\text{cm}^2$ at an Al composition of 0.22.

Figure 11 shows the total tunneling contact resistivity ρ_c as a function of Al composition in n^+ -AlGaIn with different donor concentration of 5×10^{18} , 1×10^{19} and $3 \times 10^{19} \text{ cm}^{-3}$. The optimum Al composition, where ρ_c becomes minimized, increases from 0.2 to 0.24 with increasing the donor concentration in n^+ -AlGaIn from 5×10^{18} to $3 \times 10^{19} \text{ cm}^{-3}$. This indicates that the tunneling current density across an n^+ -AlGaIn layer is enhanced with increasing the doping concentration in n^+ -AlGaIn. This is due to the reduced tunneling barrier thickness in n^+ -AlGaIn with an increased doping concentration. The calculated minimum ρ_c values for $N_{d2} = 5 \times 10^{18}$, 1×10^{19} and $3 \times 10^{19} \text{ cm}^{-3}$ were 4.4×10^{-6} , 1.8×10^{-6} and $6.4 \times 10^{-7} \Omega\text{cm}^2$, respectively. The results in Fig. 11 suggest that with higher donor doping in n^+ -AlGaIn, more reduced ρ_c would be achievable at increased Al composition in AlGaIn. In reality, however, there is a limit in the available doping density in AlGaIn because it is known that higher n -type doping becomes difficult in AlGaIn with higher Al composition. Therefore, the results in Fig. 11 can be used as a guideline for achieving minimum ρ_c , depending on the doping density available in the AlGaIn barrier layer.

4. Conclusion

We have analyzed electronic states in an AlGaIn/GaN/AlGaIn double heterostructure formed on a non-polar GaN substrate by solving Schrödinger equation coupled with Poisson equation. By calculating the tunneling contact resistivity from the tunneling current density across AlGaIn barrier layers, we have designed an optimum double heterostructure with a reduced ohmic contact resistivity. Simu-

lation results indicated that the tunneling contact resistivity was significantly reduced by introducing an n^+ -AlGaIn layer between an n^+ -GaN cap and an i -AlGaIn barrier layer. Minimum ohmic contact resistivities of 4.4×10^{-6} , 1.8×10^{-6} and $6.4 \times 10^{-7} \Omega\text{cm}^2$ were obtained with an n^+ -AlGaIn donor concentration of 5×10^{18} , 1×10^{19} and $3 \times 10^{19} \text{ cm}^{-3}$, respectively. These results suggest that the proposed new structure is capable of providing a contact resistivity value improved by as large as 4 orders of magnitude, compared to the conventional AlGaIn/GaN structure without an n^+ -AlGaIn layer.

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