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Investigation of the Polarization-Induced Charges in Modulation-Doped Al_x- $Ga_{1-x}N$/ GaN Heterostructures through Capacitance-Voltage Profiling and Simulation

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1. Introduction

Presently, $Al_xGa_{1-x}N$/GaN heterostructure field-effect transistors (HFETs) for high power, high temperature, and microwave applications are being rapidly developed. The polarization-induced electric field in an $Al_xGa_{1-x}N$ layer on GaN leads to a significant increase of the sheet concentration and the narrower confinement of the two-dimensional electron gas (2DEG) in an $Al_xGa_{1-x}N$/GaN heterostructure in comparison with that in an $Al_xGa_{1-x}As$/GaAs one. Quantitative characterization of the polarization field is necessary for a better understanding of the piezoelectric and spontaneous polarization and the strain relaxation in $Al_xGa_{1-x}N$/GaN heterostructures. In this study, capacitance-voltage (C-V) method is developed to extract the polarization-induced charge in $Al_xGa_{1-x}N$/GaN heterostructures.

2. Experimental

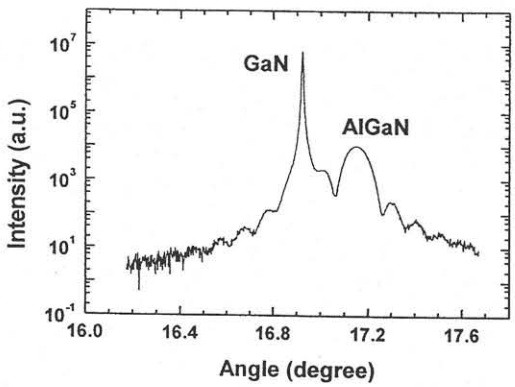

Fig.1. ω/2θ X-ray diffraction rocking curve of the modulation-doped $Al_{0.22}Ga_{0.78}N$ heterostructure with the $Al_{0.22}Ga_{0.78}N$ thickness of 45 nm. The scanning is along the GaN [0001] direction.

Three samples of high quality $Al_{0.22}Ga_{0.78}N$/GaN heterostructures were grown for this study. 2.0-μm-thick unintentionally doped GaN epilayer, an unintentionally doped $Al_{0.22}Ga_{0.78}N$ (i-AlGaN) layer, and a 25-nm-thick Si-doped $Al_{0.22}Ga_{0.78}N$ (n-AlGaN) layer were deposited successively for each sample. The thickness of the i-AlGaN layer was 5 nm for Sample 1, 20 nm for Sample 2, and 50 nm for Sample 3. Fig. 1 is the ω/2θ X-ray diffraction rocking curve of Sample 3. Ohmic contact using Ti/Al/Pt/Au multilayers and Schottky contact using Pt/Au bilayers were fabricated on the sample surfaces, forming the structure of the Schottky diodes. C-V measurements were carried out at RT using a HP 4194A LCR meter with a frequency of 100 KHz.

2. Results and Discussion

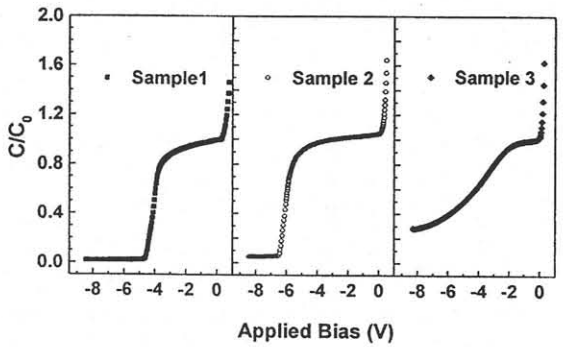

Fig. 2. Normalized C-V profiling of the three samples

Fig. 2 shows the normalized C-V profiling of the three samples. C_0 appeared in the figure is defined as:

$$C_0 = \varepsilon_0 \varepsilon_{AlGaN} A / d_{AlGaN}, \quad (1)$$

where A is the area of Schottky contacts, d_{AlGaN} is the barrier thickenss, ε_{AlGaN} is the relative dielectric constant of $Al_{0.22}Ga_{0.78}N$.

As shown in Fig. 2, when the reverse applied voltage is high, the capacitance is small and the corresponding boundary of the depletion layer is in GaN. With decreasing the reverse voltage, a capacitance plateau appears, where $C/C_0 \approx 1$, corresponding to the depletion of the 2DEG located at the heterointerface. Between the left part and the plateau, there is a transition region, where the capacitance increases rapidly with decreasing the reverse voltage. The voltage positions of the transition region in three samples are much different from each other. It is about - 4.0 V for Sample 1, - 6.0 V for Sample 2, and - 2.5 V for Sample 3. At the right of the plateau, another sharp capacitance slope (right slope) appears, indicating that the depletion layer is in $Al_{0.22}Ga_{0.78}N$. The start voltage

position of the right slope is about 0.24 V for Sample 1, 0.44 V for Sample 2, and 0.16 V for Sample 3, respectively.

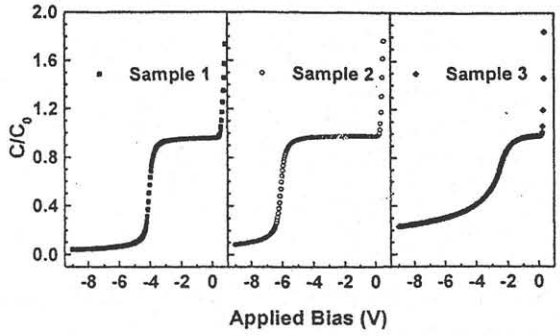

Fig. 3. Simulated C-V characteristics of the three samples

Numerical simulation was made based on the experiment results. The three-dimensional Fermi model was used. According to the simulation, the position of the transition region and the position of the right slope in every curve are determined by the polarization field, the barrier height ϕ_b, and the doping profiles of the n-AlGaN layer. The polarization field at the heterointerface influences the position of the transition region remarkably, but influences the position of the right slope slightly. Meanwhile, ϕ_b and the doping level of n-AlGaN influence both the positions of the transition region and the right slope remarkably. Thus, the polarization field can be extracted when the positions of the transition region and right slope in the simulated C-V curve both agree with those in the measured C-V curves. The simulated C-V curves of the three samples are shown in Fig. 2. They fit the measured curves well. The parameters extracted from the simulation are listed in Table I.

Table I. The parameters derived from the simulation, including the Pt/$Al_{0.22}Ga_{0.78}N$/GaN Schottky barrier height ϕ_b, the donor concentration in n-AlGaN N_{d1}, the donor concentration in GaN N_{d2}, and the sheet density of the polarization-induced charges N_p.

Sample No.	ϕ_b (eV)	N_{d1} (cm^{-3})	N_{d2} (cm^{-3})	N_P (cm^{-2})
1	1.2	$1.51x10^{18}$	$1.0x10^{16}$	$6.78x10^{12}$
2	1.2	$1.51x10^{18}$	$1.0x10^{16}$	$6.78x10^{12}$
3	1.2	$1.51x10^{18}$	$6.0x10^{16}$	$1.30x10^{12}$

N_P at an $Al_xGa_{1-x}N$/GaN heterointerface is determined by both the spontaneous and piezoelectric polarization of $Al_xGa_{1-x}N$:

$$N_P(x) = N_{SP}(x) + N_{PE}(x), \quad (2)$$

where x is the mole fraction of Al in $Al_xGa_{1-x}N$, and N_{SP} and N_{PE} are the sheet charge density induced by spontaneous and piezoelectric polarization, respectively. N_{SP} is determined by x, and N_{PE} can be expressed as:

$$N_{PE}(x) = N_{PE\max}(x)(1-R) \quad (3)$$

where $N_{PEmax}(x)$ is the piezoelectric polarization-induced sheet charge density when the $Al_xGa_{1-x}N$ layer on GaN is unrelaxed, and R is the lattice relaxation ratio of an $Al_xGa_{1-x}N$ layer on GaN. When the $Al_xGa_{1-x}N$ thickness is less than the critical thickness, the strain in the barrier is unrelaxed, and thus $R = 0$. When the $Al_xGa_{1-x}N$ barrier is thicker than the critical thickness, the strain in the barrier is partially relaxed or fully relaxed, and thus $R>0$. In this case, R increases with increasing the barrier thickness.

The simulation suggests that R is equal for Sample 1 and Sample 2, which are different in barrier thickness. Therefore, we think that the $Al_{0.22}Ga_{0.78}N$ thickness is below the critical thickness in these two samples. We think the $Al_{0.22}Ga_{0.78}N$ layer in Sample 3 is partially relaxed. Since the strain in $Al_{0.22}Ga_{0.78}N$ becomes much weaker, the density of the polarization-induced charges becomes much lower in Sample 3 than in Sample 1 or Sample 2.

4. Conclusions

C-V measurement and simulation were performed to investigate the polarization-induced sheet charge density in $Al_xGa_{1-x}N$/GaN heterostructures. The simulation based on the experimental results indicates that the sheet density of the polarization-induced charges at the heterointerface is 6.78 x 10^{12} cm^{-2} in the samples with the $Al_{0.22}Ga_{0.78}N$ thickness of 30 nm or 45 nm. The charge density reduces to 1.30 x 10^{12} cm^{-2} in the sample with the $Al_{0.22}Ga_{0.78}N$ thickness of 75 nm. It is thought that the reduction of the polarization-induced charges at the heterointerface is due to the partial relaxation of the $Al_{0.22}Ga_{0.78}N$ layer on GaN.

Acknowledgments

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