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Analysis of Band Alignment of Metal/AlGaN/GaN Structures with HXPES

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Abstract of Bachelor Thesis

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Recently, power consumption of information processing is increasing. To suppress the increase, high efficiency transistor and power converter are needed and expected to be assumed by the AlGaN/GaN HEMT. However, there are many problem to be implemented such as gate leakage current, current collapse and decrease of reliability. The defect of AlGaN surface caused by process for manufacturing is assumed one of the causes of these problems. However, under the circumstances, sufficient measurement does not found.

In this thesis, measurement of defect of AlGaN surface in AlGaN/GaN HEMT is proposed. Therefore, the purpose of this thesis is to estimate the distribution of AlGaN surface defect by Current-Voltage measurement and High X-ray photoelectron spectroscopy (HXPES).

Some Schottky gate AlGaN/GaN HEMTs that have each different gate metal were prepared as the measured samples. Gate leakage current is measured by Current-Voltage measurement and the electron in the inner shell is measured by HXPES. As the result, Current-Voltage measurement find the difference of gate leakage current depend on the kind of gate metal and with or without annealing, HXPES analysis find the distribution of defect in AlGaN layer.

In conclusion, this measurement technique is efficient for diagnosis of surface defect suppression process in AlGaN/GaN HEMT and able to be adopted to general material of semiconductors.
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Chapter 1 Introduction

1-1 Saving energy the present circumstances need

In the present circumstances, some environmental problems, such as global warming, get more acute and cannot be ignored. On the other hand, consumption of energy per person and also in our country have been increasing. Furthermore, electricity accounts for the largest percentage of consumption of energy. So it is the most important for restraining environmental problems to use electricity more effectively and suppress consumption of energy.

1-2 New materials for power semiconductor devices

Currently, silicon is the most commonplace as the semiconductor material. However silicon power devices have already reached the limit of the physical property in reducing electric power loss, size of chip and break down voltage. Silicon is getting insufficient as the upcoming material for power semiconductor devices. On the other hand, new materials called next generation semiconductors such as GaN and SiC is receiving a lot of attention. Table 1-1 is a table that compares the physical properties of silicon and two new generation semiconductors.[1.1][1.2]

Table 1-1 Physical properties of semiconductor materials

<table>
<thead>
<tr>
<th></th>
<th>Si</th>
<th>GaN</th>
<th>4H-SiC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Band gap $E_g$ (eV)</td>
<td>1.1</td>
<td>3.4</td>
<td>3.3</td>
</tr>
<tr>
<td>Dielectric constant $\varepsilon$</td>
<td>11.8</td>
<td>9.5</td>
<td>10.0</td>
</tr>
<tr>
<td>Break down field $E_c$ (V/cm)</td>
<td>$3.0\times10^5$</td>
<td>$3.3\times10^6$</td>
<td>$3.0\times10^6$</td>
</tr>
<tr>
<td>Electron mobility $\mu_e$ (cm$^2$/Vs)</td>
<td>1500</td>
<td>3050(HEMT)</td>
<td>1000</td>
</tr>
<tr>
<td>Figure of merit(ratio against Si)[1.3]</td>
<td>1</td>
<td>957</td>
<td>565</td>
</tr>
</tbody>
</table>

Baliga’s figure of merit used in table 1-1 is expressed as $\varepsilon\mu_e E_c^3$. Electron mobility of GaN itself used in Baliga’s figure of merit is 1200 cm$^2$/Vs. [1.1,1.2]

1-3 GaN wide band gap semiconductor

Gallium nitride (GaN) is material that satisfies demands of upcoming power devices. Wide band gap prevents the electron exciting from valence band to conduction band. It induces high break down voltage specifically that is tenfold as much as silicon. Furthermore, electron mobility of GaN itself is nearly same as that of silicon, but a high electron mobility compared to silicon is realized by use of AlGaN/GaN HEMT lateral structure shown in Figure 1-1 without intentionally doping. A high density of two-
dimensional electron gas (2DEG) occurs at the AlGaN/GaN interface by piezoelectric and spontaneous polarization effects, as shown in Figure 1-2. The piezoelectric polarization is result from the stress caused by difference in lattice constant. The spontaneous polarization is result from the crystal structure of Ga-face GaN and AlGaN, as shown in Figure 1-3.

![Figure 1-1 AlGaN/GaN HEMT structure](image)

![Figure 1-2 Piezoelectric and spontaneous polarization](image)
1-4 Problems to realize high performance of AlGaN/GaN HEMTs

AlGaN/GaN HEMTs are attractive as a new power device, however there are some problems to solve in order to realize a high performance. Firstly, leakage current expressed by thermionic emission, thermionic field emission and thin surface barrier model increase at Schottky contact [1.5,1.6,1.7,1.8]. Secondly, a current collapse and low reliability occur with passivation layer [1.9,1.10]. These problem is thought to be occurred by electric trap in AlGaN surface.

1-4-1 Leakage current at Schottky contact

In the case of ideal Schottky contact, the current density is expressed as only thermionic emission formulas of Padovani and Startton

\[ J = J_s \left( \exp \left( \frac{qV}{nkT} \right) - 1 \right) \]  

(1.1)

Where

\[ J_s \equiv A^*T^2 \exp \left( - \frac{q\phi_{Bn}}{kT} \right) \]  

(1.2)
Where $A^*$ is effective Richardson constant. $T$ is the absolute temperature, $q$ is electronic charge. $\Phi_{Bn}$ is Schottky barrier height. $k$ is Boltzmann’s constant. $V$ is applied voltage. $n$ is ideality factor.

Equation (1.1) is similar to the transport equation for p-n junctions with the exception of the saturation current densities. However, under the reverse bias current got by actual survey is extremely huge. It is the leakage current and augments electricity consumption. Electron tunneling caused by surface donors related to nitrogen vacancy is suggested to be the origin of leakage current. So leakage current is expressed by not only thermionic emission, but also thermionic field emission. Furthermore thin surface barrier model is also proposed.

1-4-2 Current collapse

AlGaN/GaN HEMT have a cumbersome problem called current collapse. It is denoted that on-resistance increase when high voltage is applied. It is assumed that current collapse is caused by surface defect. When high voltage is applied, electrons trap to surface defect from two dimensional gas. It causes the increase of resistance. Figure 1-4 shows mechanism that two dimensional gas decrease.

![Figure 1-4 Mechanism of current collapse](image)

(a) without gate voltage
(b) high gate voltage applied [1.11]
1-5 Purpose of this study

In this thesis, the distribution of surface defect that cause the serious problems such as the leakage current and the current collapse is estimated by two approaches. One is the I-V measurement, the other is XPS. This chapter, each chapter is described about construction and contents of this thesis.

In chapter 1, power devices requirement, feature of AlGaN/GaN HEMT and problem.
In chapter 2, fabrication process and characterization methods are described, which relate to chapter 3 and chapter 4.
In chapter 3, result of I-V measurement is shown and it discloses the more or less of the surface defect.
In chapter 4, result of HXPES measurement is shown and it discloses the distribution of donor accrued from defect in AlGaN.
In chapter 5, summarizes in this study.
Figure 1-5 shows the contents of this thesis, which is consisted of 5 parts.
References


Chapter 2 Fabrication and Characterization

2-1-1 Fabrication procedure of Current-Voltage measurement

Figure 2-1 shows fabrication procedure of samples for I-V measurement. The undoped AlGaN/GaN heterostructure used in this work was grown by epitaxial growth. To clean the surface of AlGaN, acetones and ethanol are used. The substrate was soaked in
acetones and subjected to ultrasonic cleaning in 2 min. It was soaked in ethanol for cleaning acetones. For device isolation, lithography and mesa etching was performed by Reactive Ion Etching (RIE) with Cl\textsubscript{2}. The mask pattern of contact electrode on the substrate was formed by lift-off method. The source and drain electrodes were formed by RF magnetron sputtering process. These metals were sputtered in order of Ti, Al, Mo and TiN at the surface of AlGaN. Then, rapid thermal annealing (RTA) at 950 °C for 1 min in nitrogen was performed and ohmic characterization was confirmed between source electrode and drain electrode. The mask pattern of gate electrode was also formed by lift-off method. Four kinds of gate electrodes Al, W, TiN and Ni were sputtered 50 nm. Finally, RTA at 300 °C for 10 min in F.G. ambient was performed.

Figure 2-1 Fabrication process outline of Current-Voltage measurement

2-1-2 Fabrication procedure of HXPES measurement

Figure 2-2 shows fabrication procedure of samples for HXPES measurement. The undoped AlGaN/GaN substrate is same condition as used in I-V measurement. To clean
the surface of AlGaN, SPM cleaning and HF treatment were provided. Schottky contacts with a thickness of 8 nm were formed at the surface of AlGaN by RF magnetron sputtering process. Ni, TiN, Al, and W were used as the Schottky contact metals. Finally, RTA at 300 °C for 10 min in F.G. ambient was performed.

2-2 Experimental principles
Below is the detail of experiments in the fabrication procedure.

2-2-1 Cleaning with acetones and ethanol
When the organic matter coat the AlGaN surface, acetones is effective to remove the organic matter. Then substrate is wash by ethanol because increasing the number of cleaning process remove more foreign matters.

2-2-2 RF magnetron sputtering process
Radio frequency (RF) magnetron sputtering is used to deposit metals. A high frequency voltage applied in low pressure Ar gas generates plasma which is consisted of electrons and Ar ions in a high energy state. Then, ionized Ar atoms are accelerated by applied voltage and supplied high kinetic energy. The accelerated Ar ions strike the surface of target which is sputtering metal. The metallic atoms supplied kinetic energy from Ar ions fly outside of target to substrate. A magnet is set underneath the target, so that the plasma is generated near the magnet. It minimizes the plasma damage to substrate. Figure 2-3 shows illustration of RF magnetron sputtering.
2-2-3 Dry etching by RIE
Reactive ion etching is used to both AlGaN

2-2-4 Rapid thermal annealing (RTA)
To decrease disarrangement and stress, rapid thermal annealing is performed at 300 °C for 10 min in forming gas ambient. Thermal diffusion approximate energy state of the crystal stable. Therefore, electric contact between metals and AlGaN is improved. To manufacture ohmic contact, RTA is also performed at 950 °C for 1 min in nitrogen ambient.

2-2-5 SPM cleaning and HF treatment
Various contaminations such as particles and organic substances are produced during semiconductor manufacturing process. They cause a decline in the adhesion between the substrate and formed thin layer. Therefore, surface cleaning is important for maintaining reliability. SPM cleaning is one of the efficient cleaning methods. SPM is the abbreviation for sulfuric acid/hydrogen peroxide mixture. The mixture ratio, sulfuric acid:hydrogen peroxide = 4:1, is often used. SPM strongly oxidizes surface layer including particles and organic substances. SPM cleaning is often taken place at 180 °C because enhances oxidizability and reproducibility. Then, HF treatment removes chemical oxidized layer including particles and organic substances formed during SPM cleaning. HF strongly corrodes the inorganic oxides. HF is made less concentrated to 1% in this treatment.
In this study, SPM cleaning was done at 180 °C for 10 min. HF treatment was done at room temperature for 1 min.
2-3 Principle of Current-Voltage measurement

Although generally $I_g-V_{gd}$ characteristic of Schottky contact is explained by thermionic emission theory, practically it is changed by the quantity and distribution of surface donor. Namely it is explained by combination of thermionic field emission theory and field emission theory. In other words, when quantity and distribution of surface donor are assumed and theoretical curve derived from field emission and thermionic field emission correspond with measured curve, it is possible to presume quantity and distribution of surface donor.

2-3-1 Thermionic emission

The thermionic emission theory is used when the Schottky barrier height $q\Phi_{Bn}$ is much larger than $kT$. In Figure 2-4(a), there is thermal equilibrium, the existence of a net current flow does not affect this equilibrium so that one can superimpose two current fluxes one from metal to semiconductor, the other from semiconductor to metal, each with a different quasi Fermi level. In Figure 2-4(b), applied voltage $V$ move Fermi level in the semiconductor upper direction. Even when some voltage applied, current from semiconductor to metal does not change because Schottky barrier height seen from metal side is constant, other current from metal to semiconductor increase. So thermionic emission is expressed as Equation(1.1).

![Figure 2-4(a) Electrons transport processes between metal and semiconductor at thermal equilibrium](image)

\[ E_F \quad \text{Metal} \quad \text{Semiconductor (n-type)} \]

\[ q\Phi_{Bn} \quad q\Phi_{bi} \quad E_C \quad E_F \]
The tunneling current can be expressed by field emission theory and thermionic field emission theory. While field emission is a pure tunneling process, thermionic field emission is tunneling of thermally excited carriers which see a thinner barrier than field emission. The relative contributions of these components depend on both temperature and doping level. A rough criterion can be set by comparing the thermal energy $kT$ to $E_{00}$ which is defined as

$$E_{00} \equiv \frac{q}{2} \sqrt{\frac{N}{m^* \varepsilon_s}} \quad (2.1)$$

Where $h$ is reduced Planck constant, $N$ is carrier density, $m^*$ is effective mass of electron, $\varepsilon_s$ is permittivity of semiconductor.

When $kT \ll E_{00}$, field emission dominates. When $kT \approx E_{00}$, thermionic field emission is the main mechanism which is a combination of thermionic emission and field emission. Under forward bias, the current due to field emission can be expressed as

$$J_{FE} = A^* T \pi e^{\frac{-q(\phi_{Bn} - V_F)}{E_{00}}} \frac{c_1 k \sin(c_1 \pi kT)}{c_1 k \sin(c_1 \pi kT)} \quad (2.2)$$

Where
c_1 \equiv \frac{1}{2E_{00}} \log \left[ \frac{4(\phi_{Bn} - V_F)}{-\phi_n} \right] \quad (2.3)

The much weaker temperature dependence here (absent in the exponential term) compared to thermionic emission which is a characteristic of tunneling. The current due to thermionic field emission is expressed by

$$J_{TFE} = \frac{A^{**} T \sqrt{\pi E_{00} q (\phi_{Bn} - \phi_n - V_F)}}{k \cos \left( \frac{E_{00}}{kT} \right)} \times \exp \left( \frac{-q\phi_n q(\phi_{Bn} - \phi_n)}{kT} \right) \exp \left( \frac{qV_F}{E_0} \right) \quad (2.4)$$

Where

$$E_0 \equiv E_{00} \coth \left( \frac{E_{00}}{kT} \right) \quad (2.5)$$

This thermionic field emission peaks roughly at energy as follow

$$E_m = \frac{q(\phi_{Bn} - \phi_n - V_F)}{\cosh^2 \left( \frac{E_{00}}{kT} \right)} \quad (2.6)$$

Where $E_m$ is measured from $E_C$ of the neutral region. Under reverse bias, the tunneling current can be much larger because a large voltage is possible. The currents due to field emission and thermionic field emission are expressed by as follow

$$J_{FE} = A^{**} \left( \frac{E_{00}}{k} \right)^2 \left( \frac{\phi_{Bn} + V_R}{\phi_{Bn}} \right) \exp \left( \frac{2q\phi_{Bn}^2}{3E_{00} \sqrt{\phi_{Bn} + V_R}} \right) \quad (2.7)$$

$$J_{TFE} = A^{**} T \sqrt{\pi E_{00} q \left[ V_R + \frac{\phi_{Bn}}{\cosh^2 \left( \frac{E_{00}}{kT} \right)} \right]} \times \exp \left( \frac{1q\phi_{Bn}}{kT} \right) \exp \left( \frac{qV_R}{\varepsilon'} \right) \quad (2.8)$$

Where
\[ \varepsilon' = \frac{E_{00}}{ \left( \frac{E_{00}}{kT} \right) - \tanh \left( \frac{E_{00}}{kT} \right)} \]  

(2.9)

**2-3-3 Thin surface barrier model**

Recently, an entirely different model called the thin barrier model (TSB) is proposed. In metal-GaN contact or metal-AlGaN contact, simply thermionic field emission and field emission model cannot explain the measured leakage current especially when reverse bias is applied. It is assumed that the width of the Schottky barrier is reduced by the existence of donors due to surface defect, and that field emission or thermionic field emission through the thin surface barrier region gives the major current leakage path when both forward and reverse are applied. Figure 2-5(a) shows TSB model and Figure 2-5(b) shows the band diagram. It is defined that TSB regions having a thickness \( D \) as shown in Figure 2-5(a). This model can explain the tendency of the temperature dependences of the \( I-V \) curves. In Figure 2-5(b), the potential at the boundary \( x = D \) is defined as \( \Phi_D \), the potential shape in TSB region is sharp parabola, whose minimum potential is defined as \( \Phi_0 \). It is defined \( V_0 \) as the bias voltage at which \( \Phi_0 = \Phi_D \) holds, then \( V_0 \) and \( \Phi_0 \) are given by following equations.

\[ V_0 = \phi_B - \frac{qN_{DS}}{2 \varepsilon_S \varepsilon_0} D^2 - V_n \]  

(2.10)

With

\[ V_n = kT \log \left( \frac{N_C}{N_D} \right) \]  

(2.11)

For \( V < V_0 \)

\[ \Phi_0 = \frac{qN_{DS}}{2 \varepsilon_S \varepsilon_0} \left( 1 - \frac{N_D}{N_{DS}} \right) \left( \sqrt{\frac{2 \varepsilon_S \varepsilon_0}{qN_D}} (V_0 - V) + D^2 - D \right)^2 + V + V_n \]  

(2.12)

And for \( V > V_0 \),

\[ \Phi_0 = V + V_n \]  

(2.13)

The average forward saturation current density is given by the following equation.
The reverse saturation current density is given by one of the following two equations, depending on whether the thermionic field emission process or the field emission process is dominant.

For thermionic field emission

\[
J_{SR} = \eta A^* T \frac{q \sqrt{\pi E_{00}(\phi_B - \phi_0) \tanh\left(\frac{E_{00}}{kT}\right)}}{k \cosh\left(\frac{E_{00}}{kT}\right)} \times \exp\left(qV_n/kT\right) \exp\left[q(\phi_B - V_n)/n_F kT\right]
\]  

(2.14)

For field emission

\[
J_{SR} = \eta A^* T \frac{\pi E_{00} \exp\left[-2q \phi_B^2 3 E_{00}q(\phi_B - \phi_0)\right]}{k \left[\frac{\phi_B}{\phi_B - \phi_0}\right]^2 \sin\left[\frac{\pi k t \left[\frac{\phi_B}{\phi_B - \phi_0}\right]^2}{E_{00}}\right]} \]  

(2.15)

(2.16)

Here, \(\eta\) is denoted the ratio of the total TSB area to the total area of Schottky contact. The reverse ideality factors satisfied the following relation.

\[
n_R = \frac{N_{DS}}{N_D} \frac{1}{(1 - n_F)}
\]  

(2.17)
2-4 Principle of HXPES measurement

Hard X-ray photoelectron spectroscopy (HXPES) is one of the most effective method of determining the elements, which composing the sample. HXPES spectra are obtained by irradiating a material with a beam of X-rays while simultaneously measuring the kinetic energy $E_k$ and number of electrons, which escape from the material being analyzed. The relation of energies is expressed as following formula.

$$hν = E_k + E_b + Φ \ (2.18)$$

Where $h$ is Planck’s constant, $ν$ is the frequency of vibration, $hν$ is incident energy, $Φ$ is work function of sample. Kinetic energy of electron is measured from Fermi level to simplify comparison among samples and $Φ$ is negligible.
The essence of XPS is measurement of binding energy $E_b$ of the electron. The distribution of change of binding energy corresponds to the distribution of the donor caused by defect in AlGaN. The measured data is convolution of each binding energy in micro area. The distribution of donor is estimated by reproducing each binding energy in micro area[2.1].

The measured photoelectron is expressed by the following formula.

$$J(E) = \int_0^{\infty} e^{\frac{-z}{\lambda \sin \theta}} \sin \theta I[E - \{E_0 + \psi(z)\}] dz \quad (2.19)$$

Where $I(E - E_0)$ is spectrum wave pattern that has the peak at $E_0$, $\psi(z)$ is electric potential profile in AlGaN, $\theta$ is take-off angle, $\lambda$ is IMFP. Spectrum of each depth of micro area reduce exponentially according to the member of the equation $e^{\frac{-z}{\lambda \sin \theta}}$. Figure 2-6 is the schematic views of the reproduce measured spectrum data. In this study, the binding energy of the samples was measured by hard XPS at Spring-8 BL46XU.

**Figure 2-6 band diagram expressed by spectra**

2-4-1 **Relation between binding energy and distribution of donor**

Binding energy that correspond to the depth in AlGaN means band alignment. When donor do not exist in AlGaN, electric field in AlGaN is constant in spite of the depth because of only spontaneous polarization and piezo polarization. However existence of donor bends the band alignment and it is expressed as following formula Poisson’s equation.

$$\phi(z) = -\frac{eN_d}{2\epsilon_{AlGaN}\epsilon_0}(z + W_n)^2 \quad (2.20)$$
Where \( N_d \) is donor concentration, \( W_n \) is the end of distribution of donor from AlGaN surface.

### 2-4-2 Distribution of photoelectron

The distribution of photoelectron is expressed by Voigt function that is convolution of Gaussian function and Lorentz function. The distribution of ideal electron is expressed by only Lorentz function, but actual measurement have measurement error such as error of a spectroscopiste. Voigt function is expressed as following formula.

\[
P(x)_V = \int_{-\infty}^{\infty} L(s) G(x - s) ds \quad (2.21)
\]

Where \( L(s) \) is Lorentz function and \( G(s) \) is Gaussian function.

\[
L(s) = \frac{1}{\pi} \frac{\sigma}{(s - s_0)^2 + \sigma^2} \quad (2.22)
\]

\[
G(s) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{ -\frac{(s - s_0)^2}{2\sigma^2} \right\} \quad (2.23)
\]

In this study, for brevity Pseudo-Voigt function is cited instead of Voigt function. Pseudo-Voigt function is expressed as following formula.

\[
P(s)_{p-V} = \eta \frac{1}{\pi} \frac{\sigma}{(x - x_0)^2 + \sigma^2}
\]

\[
+ (1 - \eta) \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{ -\frac{(x - x_0)^2}{2\sigma^2} \right\} \quad (2.24)
\]

Where \( \eta \) is the ratio of Lorentz function to Pseudo-Voigt function[2.2].

### 2-4-3 Measurement conditions

The incident energy is 7938.55 eV, it was same energy that binding energy of Ni2p\(_{3/2}\) corresponds to literature data 852.7 eV [2.3].\( \theta = 80^\circ \), pass energy is 200 eV, bulk is connected to metal by conductive tape. Fermi level of bulk coincide Fermi level of metal. IMFP is 11.5 nm[2.4]. It measured at room temperature.

### References
Chapter 3

3-1 Introduction

In this chapter, current-voltage characteristic was measured. It is aim to confirm leakage current when gate electrodes are different. Four kind of metals such as Ni, W, TiN and Al 50 nm thickness electrodes are selected. Annealing temperature different conditions are examined to Current-Voltage measurement. In following Schottky devices fabrication process is shown as chapter 2-1.

3-2 Current-Voltage characteristic

Figure 3-1 shows the current-voltage characteristic with 4 kind of Schottky metals which are Ni, W, TiN and Al.
Figure 3-1 Gate leakage current-Gate voltage with annealing

It shows that each leakage currents are inconsistent. It is expected that each leakage currents are same value because of strong pinning. Pinning is the phenomenon that Schottky barrier height is fixed even if the kind of metals is different. It is assumed that pinning is caused by surface states that accrues electrical charge. However, actual measured leakage currents are different from the leakage currents expected. The difference between leakage current of TiN and Al is more than 10,000 times. It suggests that surface of AlGaN is affected in some form or other by metal sputtering process or annealing process. Figure 3-2 shows the current-voltage characteristic with four kinds of Schottky metals which are Ni, W, TiN and Al without annealing process.
Figure 3-2 Gate leakage current-Gate voltage without annealing.

It shows the Current-Voltage characteristic that is similar to the one with annealing process. The difference between leakage current of TiN and Al is also more than 10,000 times. Figure 3-3 shows the Current-Voltage characteristic of all data: Ni, Al, TiN, Al, with or without annealing.
In Figure 3-3, the solid lines are characteristic without annealing process and dotted lines are characteristic with annealing process. It is sure that the kind of metal is more effective than the presence or absence of annealing process. The gate metals contact with only AlGaN surface. It shows that surface of AlGaN is important to understand leakage current. The surface donor caused by sputtering process is considered as the one possibility. When a surface metal generates a chemical reaction with nitrogen in AlGaN surface, nitrogen vacancy that works as a donor is generated [3.1,3.2]. The more nitrogen vacancies present, the more leakage current flows because of electron tunneling.

1.00E-10
1.00E-09
1.00E-08
1.00E-07
1.00E-06
1.00E-05
1.00E-04
1.00E-03
1.00E-02
1.00E-01
1.00E+00
1.00E+01
1.00E+02
-6 -5 -4 -3 -2 -1 0 1
Gate Leakage Current (A/cm²)
Gate Voltage (V)

**3-3 Conclusion**

In order to confirm the current-voltage characteristic, Schottky diode is prepared on condition that some kind of gate metal is used. Then, in the case of Schottky gate, leakage currents depend on the kind of metal in spite of strong pinning between metal and AlGaN surface. Presence or absence of annealing has less impact to the leakage current than the kind of metal. It is assumed that the impact metal sputtering on AlGaN surface is important to understand the leakage current.
References

Chapter 4
4-1 Introduction
In this chapter, binding energy of electron in AlGaN is measured by HXPES. In this study, it is aim to analyze and estimate quantity and distribution of donor caused from nitrogen vacancy in AlGaN. Four kind of metals such as Ni, W, TiN and Al 8nm thickness electrodes are selected. In following Schottky sample fabrication process is shown as chapter 2-2, measurement condition is shown as chapter 2-4-3.

4-2 Measured spectrum
HXPES measurement is used to learn detail state of inside of AlGaN. Figure 4-1 shows Al1s spectrum of Ni that is annealed at 300 °C for 10 min in forming gas. The data measured by HXPES is kinetic energy of photoelectron. For deriving binding energy of electron, measured kinetic energy is subtracted from incident energy shown as chapter 2-4. The incident energy is 7983.55 eV. It is derived by coinciding measured spectrum peak of Ga2p2/3 and literature data of spectrum of Ga2p2/3 852.7 eV.
Figure 4-1 Measured spectrum of Ni Schottky

Figure 4-1 illustrates the lacking symmetry with the peak of measured spectrum. If the energy band of AlGaN do not bend, measured spectrum will be symmetry. However, left side that express high binding energy of actually measured spectrum is broader than right side. It means that binding energy becomes higher as deep AlGaN is measured. In this connection, IMFP of AlGaN is 11.5 nm and Al1s at three times deep as IMFP can be detected by HXPES. Figuer 4-2 shows the most coincided theoretical curve if band of AlGaN is bent by only constant electric field caused by piezo polarization and spontaneous polarization.
Figure 4-2 spectrum of Ni Schottky with constant electric field

Figure 4-2 illustrate the discordance between actually measured curve and theoretical curve derived by equation in chapter 2-4. In the left side, two lines coincide well. However, in the right side, theoretical curve is sharper than measured curve. It means the actually binding energy near the AlGaN surface is larger than assumed binding energy. In AlGaN surface, presence of donor like defect is consider as one possibility. Then the model is formed by assuming that constant donor like defect presence only from AlGaN surface to position $x$ nm with the origin located at AlGaN surface. Donor like defect increase the binding energy as Poisson’s equation expressed in chapter 2-4-1. Figure 4-3 illustrate the result of fitting of the model assuming surface donor.
Figure 4-3 (a) spectrum of Ni Schottky with constant electric field and donor (b) theoretical spectrum compose spectrum in (a)

Figure 4-3(a) shows the coincidence of measured spectrum and theoretical spectrum. Figure 4-3(b) shows the each spectrum in micro area. The distance of these peaks on the right side are broader than those on the left side. Binding energy at AlGaN surface is changed greatly. The height of each peak decrease as go the left side peaks. It shows the peaks on the left side express the binding energy of inner AlGaN. In this situation, donor density is estimated $1.8 \times 10^{19} \text{ cm}^{-3}$ and donor depth $x$ is 4.5 nm. The results of HXPES analysis of W and TiN are shown in Figure 4-4, 4-5 and Table 4-1.
Figure 4-4 (a) spectrum of TiN Schottky with constant electric field and donor (b) theoretical spectrum compose spectrum in (a)
Figure 4-5 (a) spectrum of W Schottky with constant electric field and donor (b) theoretical spectrum compose spectrum in (a)

Table 4-1 result of HXPES analysis

<table>
<thead>
<tr>
<th></th>
<th>Ni</th>
<th>W</th>
<th>TiN</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_d$ [cm$^{-3}$]</td>
<td>$1.8 \times 10^{19}$</td>
<td>$3.3 \times 10^{19}$</td>
<td>$1.2 \times 10^{19}$</td>
</tr>
<tr>
<td>$x$ [nm]</td>
<td>4.5</td>
<td>3.0</td>
<td>4.2</td>
</tr>
</tbody>
</table>
There are the differences of donor distribution among some kind of gate metals. The order of donor density analyzed in this chapter coincides the order of leakage current measured in chapter 3. It has been reported that AlGaN surface of Ni Schottky gate AlGaN/GaN HEMTs have $1.0 \times 10^{19}$ cm$^{-3}$ donor density near the analyzed quantity[4.1].

4-3 Band alignment of AlGaN

Figure 4-6 shows the band alignment derived by result of HXPES analysis.

Figure 4-6 band alignment of Ni/AlGaN/GaN structure

In the Ni, Fermi level correspond conduction band. At the interface of Ni and AlGaN, Schottky barrier height is strongly pinning and it is 1.25 eV [4.2]. AlGaN surface have donor like defect and its donor density is estimated $1.8 \times 10^{19}$ cm$^{-3}$ and distribution depth is 4.5 nm from surface of AlGaN. Total increase of energy of conduction band in AlGaN is 1.59 eV derived by HXPES analysis. At the interface of AlGaN and GaN, gap of electron affinity is 0.40 eV [4.3].

4-4 Conclusion

In order to confirm the binding energy of electron in AlGaN, metal/AlGaN/GaN sample is prepared on condition that some kind of metal is used. Then, only constant electric field cannot explain measured spectrum whatever the kind of metal is. When surface donor is assumed, actually measured curve and theoretical curve correspond well.
Therefore the difference of quantity of surface donor is revealed and its order is same as the order of leakage current explained in chapter 3. Finally, current band alignment is derived.

References

Chapter 5 Conclusions

In this thesis, we studied surface donor like defect in AlGaN. In this chapter, the studies are summarized below.
In chapter 1, the cause of serious problem such as leakage current and current collapse is surface donor like defect in AlGaN. Therefore, the method of evaluating surface donor is needed.
In chapter 2, new evaluating method is supposed.
In chapter 3, the difference of leakage current among some kinds of metals in spite of strong pinning is revealed. It indicate that metal/AlGaN surface is important to understand leakage current.
In chapter 4, finally, distribution of donor like defect is revealed by HXPES analysis. The tendency of leakage current and donor distribution is related. Current band alignment is derived by HXPES.

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Kazuki Ohga
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