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# Characterization of Ni/GaN(0001) Interfaces by Photoemission Measurements

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**Abstract**

**Chemical bonding features at the interface between EB evaporated Ni and wet-cleaned homo-epitaxial GaN(0001) have been directly evaluated by using x-ray photoelectron spectroscopy (XPS). Determination of energy band alignment and inner potential change at Ni/GaN interface have been demonstrated.**

## 1.Introduction

A clear insight into the relationship between the chemical structure and energy band alignment at the metal/GaN interface is essential to precisely control the carrier transport such as the ohmic contact and Schottky barrier height. Schottky contact of Ni/n-GaN structure have been often studied from electrical properties. And also, X-ray photoelectron spectroscopy (XPS) is one of the powerful tools to evaluate not only the chemical states but also energy band structure of stacked structure with thin films [1-3]. In this work, to get an better understanding the chemical bonding features and energy band alignment at Ni/GaN interface, XPS analysis of ultrathin Ni/n-type GaN(0001) has been performed.

## 2. Experimental Procedure

A ~2 μm-thick n-type GaN(0001) with a Si concentration of $4\times10^{16}$ $cm^{-3}$ was grown on a free-standing GaN substrate by MOCVD. Wet-chemical cleaning of the GaN(0001) surface by 36% HCl solution at 80 ºC for 20 minutes and subsequent pure-water rinse were performed to remove the surface native oxide and contaminants. From the XPS analysis, a decrease in the native oxide thickness down to ~0.2 nm and Cl atoms with an areal density of around $1\times10^{15}$ $cm^{-2}$ on the surface after the cleaning were observed [4]. Then, an Ni thin layer with a thickness of ~2 nm was deposited on the cleaned GaN surface by EB evaporation at the base pressure of $2\times10^{-7}$ Torr, After that, XPS measurements utilizing monochromatized AlKα radiation (hν = 1486.6 eV) were carried out without air exposure.

Surface topographic AFM images for the samples before and after Ni deposition shows no remarkable change in the root mean square (RMS) roughness, and uniform coverage of Ni thin layer deposited on GaN surface was confirmed (as shown in Fig. 1).

## 3. Results and Discussion

Figure 2 shows N 1s and Ga $2p_{3/2}$ spectra for the samples before and after Ni deposition on wet-cleaned GaN(0001) surface. A significant change in the N 1s signals of Ga-N bonding units originating from GaN substrate by the Ni deposition was hardly detected. On the other hand, Ga LMM Auger electron and Ga $2p_{3/2}$ signals in the lower binding energy side from Ga-N bonding units were slightly increased.

These results can be interpreted in terms that the less electronegative Ni atoms (χNi = 1.91 : Pauling units) are coordinated with the Ga atoms in the Ga-N bonding units at GaN(0001) surface (χGa = 1.81, χN = 3.04). In other words, Ga-Ni bonding units were formed at Ni/GaN interface. In addition, an amount of Ga-Ni bonding units was crudely estimated to be around 0.3 nm as an average thickness from an integrated intensity ratio of Ga-Ni to Ga-N signals in Ga $2p_{3/2}$ spectra. From Ni $2p_{3/2}$ spectrum for the sample after Ni deposition as shown in Fig. 3(a), metallic Ni component was clearly detected although the thickness of Ni layer was as thin as ~2 nm. It should be noted that Cl 2p signals were increased after Ni deposition, which suggests the diffusion and incorporation of Cl atoms into Ni layer from GaN surface during the Ni deposition.

Then, photoelectron take-off angle dependence of Ni $2p_{3/2}$, N 1s, and Cl 2p spectra for the sample after Ni deposition were measured to evaluate the depth profiling of Cl atoms and chemical structure in the sample (as shown in Fig. 4). In Fig. 4, photoelectron intensity was normalized by Ni $2p_{3/2}$ signals from metallic Ni components. Ni $2p_{3/2}$ signals from Ni oxide and Cl 2p signals were significantly increased by a decrease in the photoelectron take-off angles from 90º to 30º for surface sensitive measurements, which implies the formation of Ni oxide on the Ni layer and the incorporation of Cl atoms (~6 at.%) into NiO/Ni stack. In contrast, the N 1s and Ga Auger electron signals from the GaN substrate were decreased. From these results, a remarkable interfacial reaction between Ni and GaN(0001) hardly occurs during Ni deposition, resulting in the formation of abrupt Ni/GaN interface.

To determine the energy band alignment for Ni/GaN(0001) interface, valence band spectra for the sample after Ni deposition were measured at photoelectron take-off angle at 90º and 15º. Firstly, valence band signals from Ni/GaN(0001) were extracted by the subtraction of the signals measured at the angle of 15º from the signals at 90º

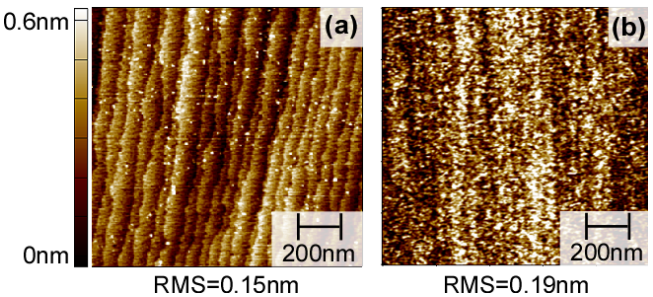


Fig. 1. AFM topographic images taken for GaN(0001) surface after (a) wet-chemical cleaning by HCl solution and (b) a ~2 nm-thick Ni deposition by EB evaporation.

after the intensity normalization by Ni oxide component (Fig. 5(a)). Then, extracted valence band signals were deconvoluted into two components originated from Ni and GaN using reference signals of Ni layer, which was separately measured for EB evaporated Ni after the removal of surface oxide by $Ar^+$ ion sputtering (Fig. 5(b)). From the energy separation of the tops of the deconvoluted valence band spectra, the valence band offset at Ni/GaN(0001) interface was obtained to be 2.40 ± 0.05eV. Based on the measured valence band offset and reported band gap value of GaN (3.40 eV) [5], the Schottky barrier height at the Ni/GaN(0001) interface was found to be 1.00 ± 0.05 eV. Moreover, vacuum level of Ni was estimated to be 0.76 eV higher than that of GaN using the reported Ni work function and GaN electron affinity [6, 7], which responsible for the inner potential change due to the electrical dipole moment at Ni/GaN interface.

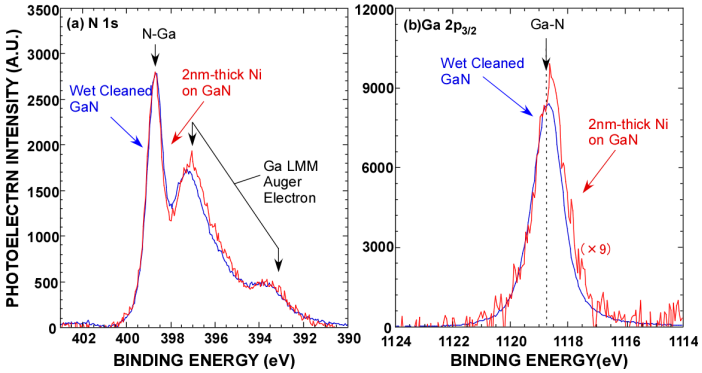


Fig. 2. (a) N 1s and (b) Ga $2p_{3/2}$ spectra for the samples before and after the Ni deposition. These spectra were measured at photoelectron take-off angle of 90º. In each spectrum, photoelectron intensity normalization and binding energy calibration were made by N 1s signals from Ga-N bonding units at 398.7 eV .

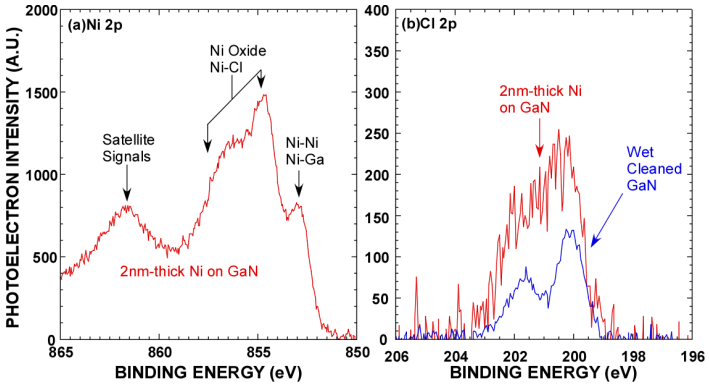


Fig. 3. (a) Ni $2p_{3/2}$ and (b) Cl 2p spectra for the samples shown in Fig. 2.

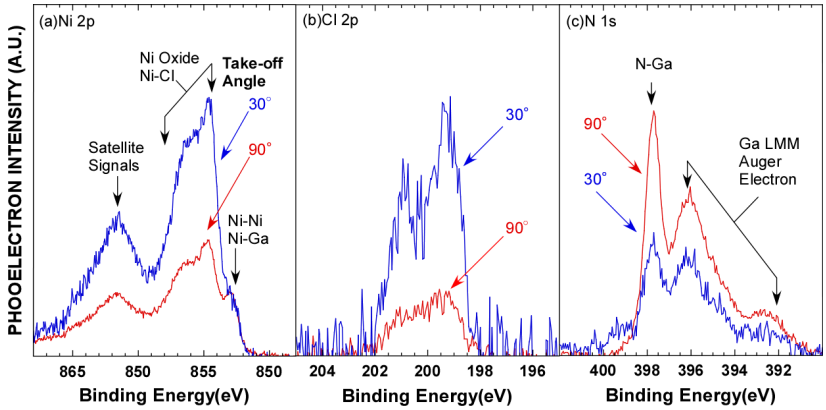


Fig. 4. (a) Ni $2p_{3/2}$, (b) Cl 2p, and (c) N 1s spectra for the sample after the Ni deposition measured at the photoelectron take-off angles of 90º and 30º. In each spectrum, photoelectron intensity normalization and binding energy calibration were made by Ni $2p_{3/2}$ signals from metallic Ni components at around 853 eV.

## 4. Summary

Abrupt Ni/GaN(0001) interface with 1~2 monolayer thick Ga-Ni bonds were formed after the EB deposition of Ni on wet cleaned GaN surface. Cl atoms remaining on GaN surface after the cleaning using HCl solution were diffused and incorporated into Ni layer during the deposition. Schottky barrier height and inner potential change at the Ni/GaN(0001) interface was found to be 1.00 eV and 0.76 eV, respectively.


## Acknowledgements

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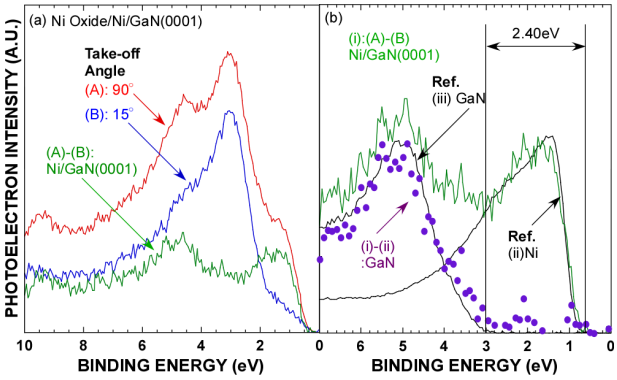


Fig. 5. (a) Measured and (b) deconvoluted valence band spectra taken for the sample after Ni deposition.

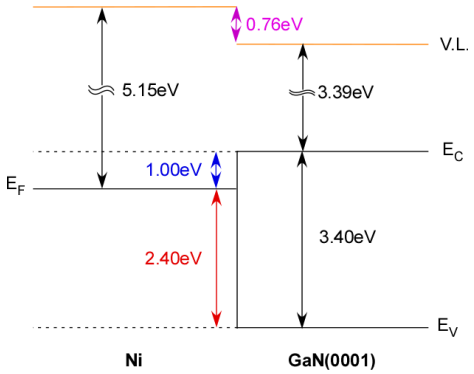


Fig. 6. Energy band alignment for Ni/GaN(0001) interface.