Band discontinuity at the interface of rutile Ti_{1-x}Co_xO_{2.8}/*p*-GaN heteroepitaxial structure studied by synchrotron-radiation photoelectron spectroscopy

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Introduction

In the field of spintronics, ferromagnetic diluted magnetic semiconductors (DMSs) are key materials. The rutile and anatase polymorphs of Co-doped TiO₂ (Ti_{1.} $_x$ Co_xO_{2.8}) are among the most extensively studied ferromagnetic DMSs because of their extremely high Curie temperature (> 400 K) and excellent transparency in the visible region.

When applying $Ti_{1,x}Co_xO_{2,\delta}$ to spintronic devices, such as the spin injection electrode and integrated optical isolator, the material has to be grown heteroepitaxially on group IV or group III-V semiconductors (Si, GaAs, etc.), which are widely used in conventional electronics. To date, however, $Ti_{1,x}Co_xO_{2,\delta}$ has been synthesized mostly on oxides, including LaAlO₃, SrTiO₃, and Al₂O₃, and heteroepitaxial growth of $Ti_{1,x}Co_xO_{2,\delta}$ on such semiconductors has scarcely been attempted.

Recently, we report the heteroepitaxial growth of roomtemperature ferromagnetic rutile $Ti_{1,x}Co_xO_{2,\delta}$ films on wurtzite GaN by pulsed laser deposition (PLD) method [1]. The high-resolution cross-sectional transmission electron microscope images of the film showed atomically smooth interface without intermixing. Thus, $Ti_{1,x}Co_xO_{2,\delta}$ is a good candidate for a spin injector in GaNbased spin-electronic devices.

In this study, expecting an application for a spinpolarized LED, the band discontinuity in the interface of $\text{Ti}_{1-x}\text{Co}_x\text{O}_{2.\delta}/p$ -GaN was evaluated with synchrotronradiation x-ray photoelectron spectra (SRPES).

Experiment

 $Ti_{0.97}Co_{0.03}O_{2.\delta}$ films were fabricated on Mg-doped *p*-type ($n_{hole} = 4 \times 10^{17}$ cm⁻³) GaN(0001)/Al_2O_3(0001) templates by PLD[1]. In order to obtain clean surfaces, GaN templates were degreased by ultrasonication in ethanol and acetone, and subsequently etched in 36% HCl solution and rinsed with deionized water. In addition, the substrates placed into the deposition chamber were preheated at 700°C in vacuum. The substrate temperature and oxygen partial pressure were keep at 550°C and 1×10⁻⁵ Torr during the deposition. The film thicknesses were 3nm and 30nm. The SRPES of the samples were measured at the Photon Factory BL-2C of KEK. The photon energy of the synchrotron radiation was 800 eV.

<u>Results</u>

Figure 1(a) shows the valence band spectra of 3 nm $Ti_{0.97}Co_{0.03}O_{2.\delta}$ on *p*-GaN. The spectra of 30 nm $Ti_{0.97}Co_{0.03}O_{2.\delta}$ film and *p*-GaN substrate were also shown in fig. 1(b) with relative binding energies which were evaluated from O1s spectra of $Ti_{0.97}Co_{0.03}O_{2.\delta}$ and N1s spectra of *p*-GaN. Comparing these valence band spectra, the difference between valence band maximum of $Ti_{0.97}Co_{0.03}O_{2.\delta}$ and *p*-GaN (Δ_{VB}) was determined as ~1.0 eV. Because the band gap of rutile TiO₂ and GaN were 3.0 and 3.4 eV, respectively, the difference between conduction band minimum (Δ_{CB}) was ~1.4 eV.

In the application of Ti_{1-x}Co_xO_{2.8}/*p*-GaN for spin LED, injecting spin-polarized electrons of Ti_{1-x}Co_xO_{2.6} to *p*-GaN is important. However, our results shows that the potential barrier for electron injection from Ti_{1-x}Co_xO_{2.6} to *p*-GaN is higher than hole injection from *p*-GaN to Ti₁ _xCo_xO_{2.6} In order to clear this problem, a tri-layer structure with a hole blocking layer would be useful.



Figure 1 Valence band spectra of Ti_{1-x}Co_xO₂₋₈/p-GaN

<u>References</u> [1] Y. Hirose *et al.*, App. Phys. Lett. 92, 042503 (2008).

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