Active and inactive dopant sites in Si-doped GaN (0001)

(D)Jingmin Tang^{1,2}, Yoshiyuki Yamashita^{1,2}

NIMS¹, Kyushu Univ²

E-mail: TANG.Jingmin@nism.go.jp

Gallium nitride (GaN) has attracted much attention because it has many excellent physical properties.¹ For GaN based devices,² Si is usually used for n-type doping. However, there is a big issue in GaN devices where the carrier concentration is much lower than the number of dopants.³ Therefore, it is crucial to analyze the chemical states and atomic structures of active and inactive dopant sites in Si-doped GaN, which introduces the knowledge that control the carrier in MOS-FET structures. In this study, the XANES and PES were used to clarify the active and inactive sites of Si-dopant in GaN.

For Si-doped GaN, the Si was doped into GaN from 0 nm to 380 nm to the surface and the concentration was 2.1×10^{20} cm⁻³, which was estimated by SIMS. XANES and PES were performed at BL1N2 and BL6N1 in Aichi synchrotron radiation center.

For Si KLL Auger spectra, the peaks at 1610.1 and 1612.2eV were observed. The peaks at 1610.1 and 1612.2 eV were assigned to SiN_x and Si_3N_4 , respectively. ^{4.5} The XANES were performed using Auger electron yield (AEY) at the Auger peaks at 1610.1(SiNx) and 1612.2 eV (Si₃N₄), which are corresponding to unoccupied states of respective SiN_x and Si₃N₄, which is shown in Fig 1. Note that E_f and CBM in Fig.1 were obtained from Si 1s core level in Si -doped GaN, N k-edge XANES and N1s spectra of undoped GaN. In Fig 1, Si₃N₄ does not have electronic states in band-gap in GaN while SiN_x exhibits the electronic states in the band-gap, indicating that SiN_x would be active dopant site in the Si-doped GaN. In order to clarify the atomic structure of SiN_x, the simulations of XANES spectra were performed using FEFF9. We found that Si atom replacing with Ga atom in Si-doped GaN could be the active dopant site in Si-doped GaN.

Key words: GaN, XANES, Si₃N₄, dopant



Fig. 1: XANES spectra of Si-doped GaN. Black solid and red solid lines indicate XANES spectra recorded by AEY at Auger components of $1612.2(Si_3N_4)$ and $1610.1 \text{ eV} (SiN_x)$, respectively.

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