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Energy-Band Offset of AlN/Diamond(111) Heterojunction Determined by X-ray Photoelectron Spectroscopy

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Abstract

The high-quality AlN epilayers were grown on hydrogen-terminated diamond (111) substrates by metal-organic vapor phase epitaxy. The electronic states and energy-band offset were evaluated by X-ray photoelectron spectroscopy. Based on the core level binding energies and valence band maximum values, valence band offset were evaluated to be 2.04 ± 0.20 eV. Bandgap energy of AlN was determined to be 6.02 ± 0.2 eV by measuring N 1*s* energy loss spectrum. The AlN/diamond heterojunction was concluded to be type-II staggered band configuration with conduction band offsets of 1.47 ± 0.2 eV.

1. Introduction

Diamond is one of the most suitable materials for high-output power and high-frequency field effect transistors (FETs), which can operate under harsh environments. Conductivity control in diamond is critically important, but it is still in the development stage. This is due to difficulties in controlling the electron and hole densities in diamond at room temperature, because of the large activation energy of dopants, such as boron (B), phosphorus, nitrogen. Therefore, a breakthrough in conductivity control for diamond-based FET devices is required to obtain high-output power and high-frequency properties. Until now, the surface channel diamond FETs using hydrogen (H2 or H)-terminated surface [1] and high-density B delta-doped diamond FETs [2] have mainly been investigated. The study on heterojunction FETs (HFETs) with diamond and different materials, such as wideband gap and ferroelectric materials, has been started by our group since ~2010 [3]. Although we have developed p-channel AlN/diamond HFETs, the problems, such as poor crystalline quality of AlN and reduction of sheet carrier density after the AlN deposition, should be overcame for the further improvement of the device performance [4]. Recently we have successfully improved the crystalline quality of AlN on diamond (111) substrates. In this study, the electronic states and energy-band offsets were evaluated by X-ray photoelectron spectroscopy (XPS).

2. Results & Discussion

High-quality AlN layers with different thickness at 5 nm and 400 nm were grown on hydrogen-terminated (H-) diamond (111) substrates by metal-organic vapor phase epitaxy (MOVPE) by means of the controlling off-angle and surface termination structure of diamond. Thermal cleaning with mixed H_2 and NH_3 atmosphere was carried out just before the AlN growth. The XPS measurements were performed by PHI Quantera SXM using a monochromated Al Kα X-ray source (hv = 1486.6 eV). All core level spectra were recorded with a 0.05 eV step and a 55 eV pass energy.

Typical results on the core level (CL) and valence band photoelectron spectra of diamond (111) and AlN are shown in Fig. 1.

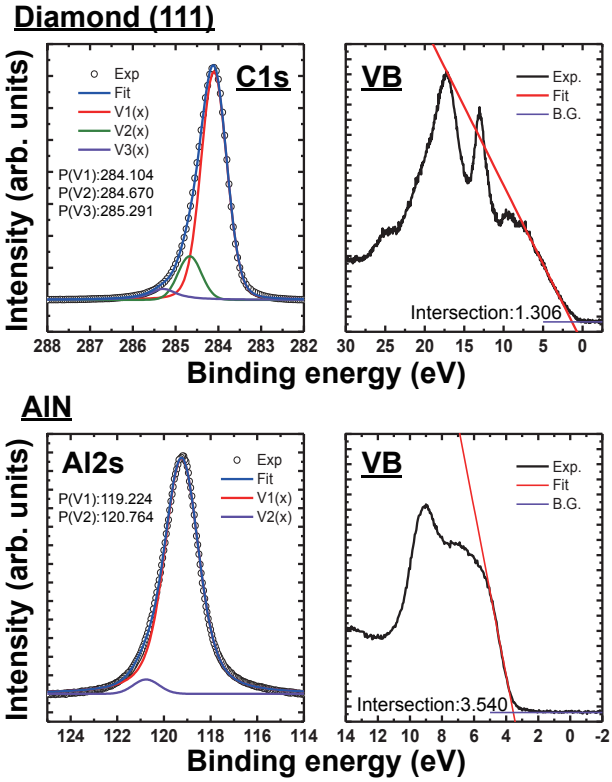

Fig. 1 C 1s core-level and VB spectra of diamond and Al 2*s* core-level and VB spectra of AlN

Based on the CL binding energies and valence band maximum (VBM) values, the valence band offset (ΔE_V) values of AlN/diamond(111) heterojunction were calculated. The used equation is below:

$\Delta E_V = (E_{CL} - E_{VBM})_{diamond} - (E_{CL} - E_{VBM})_{AlN} - \Delta E_{CL}$, (1)

where the $(E_{CL} - E_{VBM})diamond$ values are the difference in binding energy between C 1*s* CL and VBM of the diamond. The $(E_{CL} - E_{VBM})_{AlN}$ values are the difference in binding energy between Al 2*s* CL and VBM for the 400 nm thick AlN. The ΔE_{CL} values are the differences in binding energy between Al 2*s* and C 1*s* CLs for the 5 nm thin AlN. The ΔE_V values were found to be 2.04 ± 0.20 eV.

Since the energy loss of photoelectron in solids is known to be larger than the bandgap energy, the bandgap energy of AlN was evaluated by N 1*s* energy loss spectrum. The typical N 1*s* energy loss spectrum is shown in Fig. 2. The bandgap energy of AlN was determined to be 6.02 ± 0.2 eV as shown in Fig. 2.

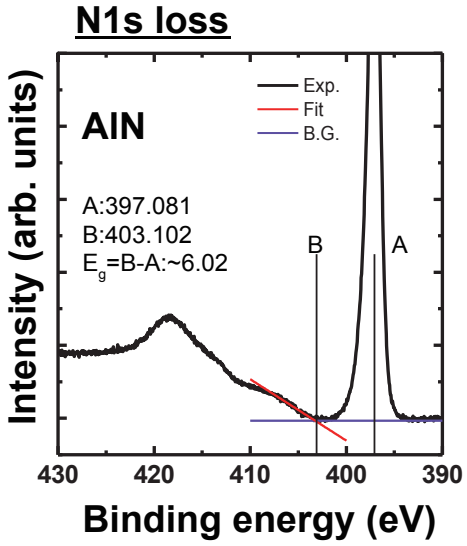

Fig. 2 N 1s loss spectrum of AlN

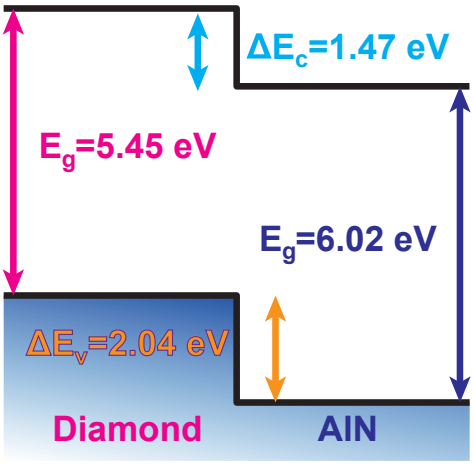

Fig. 3 Schematic illustration of energy band offset between diamond and AlN

Based on these results, the AlN/diamond heterojunction was concluded to be type-II staggered band configuration with conduction band offsets of 1.47 ± 0.2 eV. The schematics illustration of energy band offset between AlN and diamond is shown in Fig. 3.

3. Conclusions

The high-quality AlN epilayers were grown on hydrogen-terminated diamond (111) substrates by MOVPE. The electronic states and energy-band offset were evaluated by X-ray photoelectron spectroscopy. Based on the core level binding energies and valence band maximum values, valence band offset were evaluated to be 2.04 ± 0.20 eV. Bandgap energy of AlN was determined to be 6.02 ± 0.2 eV by measuring N 1*s* energy loss spectrum. The AlN/diamond heterojunction was concluded to be type-II staggered band configuration with conduction band offsets of 1.47 ± 0.2 eV.

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