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Electronic band structures of AlN/ZnO heterointerfaces studied by synchrotron radiation photoemission spectroscopy

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Introduction

AlN and ZnO have the same crystalline symmetry and the lattice mismatches between them for *a* and *c*-axies are 4.2 and 4.3%, respectively. AlN/ZnO heterostructures have large conduction band offsets (CBOs) [1], which will form a high density of 2DEG at the interfaces. However, it is difficult to suppress the formation of interfacial layer when AlN films are grown on ZnO substrates by metal organic chemical vapor deposition or molecular beam epitaxy due to their high growth temperatures. Recently, we have succeeded in growing AlN films on single-crystal ZnO substrates without forming interfacial layers by pulsed laser deposition (PLD) technique [2,3] Although the valence band offset (VBO) of (0001) *c*-plane ZnO/AlN heterojunction has been investigated using photoemission spectroscopy [4], the accurate interfacial band configurations of *c*-plane and *a*-plane AlN/ZnO are still unclear. In this study, we have investigated the electronic structures of *c*-plane and *a*-plane AlN/ZnO heterojunctions by synchrotron radiation photoemission spectroscopy (SR-PES).

Experimental

We prepared six samples in order to clarify the electronic structures of *c*-plane and *a*-plane AlN/ZnO heterointerfaces. The samples were $(000\bar{1})$ *c*-plane and $(11\bar{2}0)$ *a*-plane ZnO substrates, 4 nm thick AlN films on these substrates, and 30 nm thick AlN films. All AlN films were epitaxially grown by PLD at room temperature (RT). The SR-PES measurements were performed at the beam line BL-2C of the Photon Factory in the High Energy Accelerator Research Organization (KEK). All the core-level and valence-band photoemission spectra of the samples were measured using photon energy of 800 eV with a high-energy resolution of approximately 0.2 eV at RT. The photoemission spectra were calibrated by the position of Au Fermi level (E_F).

Results and Discussion

The schematic band diagrams for the *c*-plane and *a*-plane AlN (4 nm)/ZnO heterointerfaces and ZnO substrates are illustrated in Fig. 1. The band alignment at the interface on the ZnO side was determined by the difference in the Zn 3*p* core-level binding energy between the ZnO substrate and the AlN (4 nm)/ZnO sample. The potential on the ZnO side bends downward toward the interface for the *a*-plane AlN/ZnO heterojunction [Fig. 1(b)], while that bends upward toward the interface for the *c*-plane AlN/ZnO heterojunction [Fig. 1(a)]. This phenomenon can be explained well by the effect of spontaneous polarization (P_{SP}). The effect of piezoelectric polarization is excluded since the stains in the AlN films on ZnO substrates are almost relaxed. Because the P_{SP} of AlN and ZnO are -0.081 and -0.056 C/m^2, negative charges are induced at the *c*-plane AlN/ZnO heterointerface, which makes the potential of the ZnO side bend upward. On the other hand, for the *a*-plane AlN/ZnO heterojunction, the spontaneous polarization directions of AlN and ZnO are parallel to the interface plane. Thus, P_{SP} of AlN and ZnO do not affect the potential variation of the ZnO side across the *a*-plane interface [5].

References

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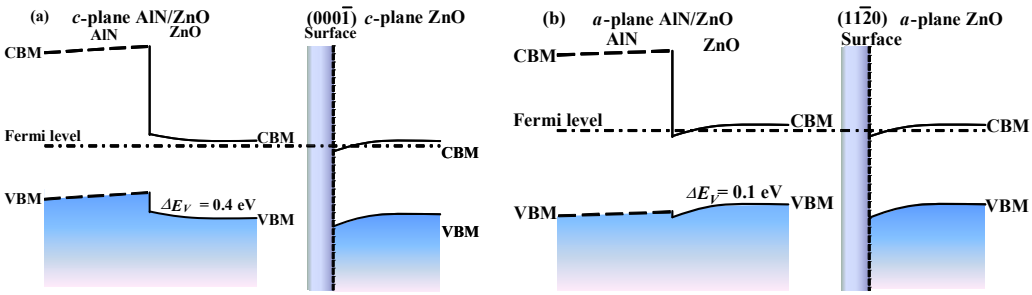

Fig. 1. Schematic band diagrams for (a) *c*-plane AlN/ZnO heterointerface and ZnO substrate, and (b) *a*-plane AlN/ZnO heterointerface and ZnO substrate