

Polarization-Induced Band Alignments at Anion- and Cation-Polar InN/GaN Interfaces

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The precise determination of III-nitride band alignment is very important for the design and characterization of III-nitride-based optoelectronic and electronic devices. Most of the reported valence-band offsets (VBOs) for the III-nitride heterojunction system show a wide disparity that might be related to the strong piezoelectric and spontaneous polarization effects. By using synchrotron-radiation photoelectron spectroscopy (PES), we demonstrate that the existence of spontaneous polarization discontinuity at the polar InN/GaN interfaces can lead to large core-level shifts and modification of their apparent VBOs. InN/GaN heterojunctions as well as InN and GaN bulk epilayers were grown along the polar *c* or *-c*-axis on Ga-face GaN/Al₂O₃(0001) and N-face AlN/ β -Si₃N₄/Si(111) growth templates by plasma-assisted molecular-beam epitaxy using a monolayer-abrupt strain relaxation technique.

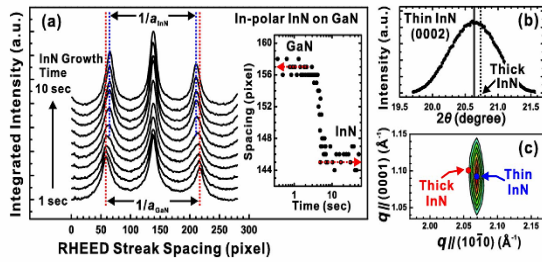


Figure 1. Structural and strain properties of thin (~6 nm thick), In-polar InN(0001) epilayer grown on a thick, fully relaxed GaN(0001)/sapphire.

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A accurate determination of the lattice parameters (*c* and *a*) and the epilayer strain states in heterojunction samples was performed by *ex-situ* synchrotron-radiation x-ray diffraction (XRD) measurements. The dotted line in the θ - 2θ scans across InN(0002) peak, shown in Fig. 1(b), marks the peak position (c_0) of a thick (~2 μ m), fully relaxed In-polar InN epitaxial film. For the case of thin, N-polar InN(000-1) epilayer, the measured *c* value is 5.718 Å. The *c*-axis strain $\epsilon_3 = -v\epsilon_1$ in thin InN epilayers (about 0.4% and 0.2% for In-polar and N-polar InN thin layers, respectively) is very uniform.

All samples studied were treated with dilute HCl etching followed by an *in-situ* anneal process (350 °C for 30 mins). In the best fit, the deconvoluted In 4*d* core-level spectra indicate a combination of a main peak from the bulk derived feature (B) and an additional component from the surface state (S), which is a signature of InN epilayers with clean surfaces (Fig. 2). The binding energy shown here has been scaled with respect to the positions of valence-band maximum (VBM) (E_V), which are obtained by linear extrapolation of the valence-band

spectra. By aligning the VBM positions of both types of InN/GaN heterojunctions, it can be clearly seen that there exists a large binding energy difference of 0.51 eV between Ga 3*d* and In 4*d* core-level emissions.

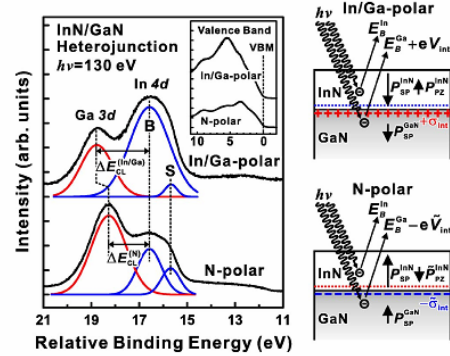


Figure 2. Ga 3*d* and In 4*d* core-level spectra of In/Ga-polar and N-polar InN/GaN heterojunctions.

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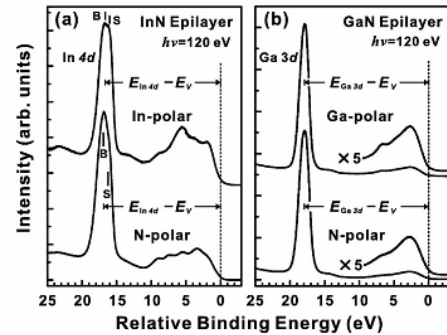


Figure 3. Photoelectron spectra of (a) InN and (b) GaN bulk epilayers with In/Ga and N polarities for InN/GaN heterojunction valence-band offset measurements.

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The VBO values can be determined by the relation of $\Delta E_V = (E_{In4d} - E_V)_{InN} - (E_{Ga3d} - E_V)_{GaN} + (\Delta E_{CL})_{InN/GaN}$, resulting in type-I VBOs of 1.04 and 0.54 eV for the In/Ga-polar and N-polar heterojunctions, respectively. In summary, we have confirmed that the polarization discontinuities across the polar III-nitride heterojunctions can be exploited to control their valence-band alignments. Large Ga core-level shifts, resulting from the interface dipoles, have been measured on In/Ga- and N-polar InN/GaN heterojunctions with monolayer abrupt, nearly fully relaxed lattices. This discovery may lead to, besides the conventional band gap engineering, an alternative degree of freedom in the design of group-III nitride heterostructure devices.