Band Alignment at Cubic (111) ScN / Wurtzite (0001) GaN Heterojunction

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With the invention of efficient blue LEDs, laser diodes, RF power amplifiers, and acoustic wave resonators for 5G-6G technologies, group III nitride semiconductors have revolutionized the electronic and photonics industry. ScN is a promising dislocation reduction buffer bridge between cubic Si and wurtzite GaN systems that can act as a current-spreading layer. As a transition metal nitride semiconductor, ScN has the potential to bring thermoelectric, plasmonic, spintronic, high piezo, and ferroelectric properties to GaN, making it essential to study its electronic structure.

This work reports a direct measurement of the valance band offset of (111) ScN/ (0001) GaN heterojunction. Twin cubic (111) ScN films of different thicknesses were epitaxially grown on (0001) oriented metal polar GaN substrates using nitrogen plasma molecular beam epitaxy (MBE), as indicated in Fig. 1a. Reflection high energy electron pattern of grown ScN film, as shown in Fig. 1b, confirms the twin cubic growth of ScN films. The MBE-grown (111) cubic ScN film has less than 0.1 % in-plane lattice mismatch with the wurtzite (0001) GaN as shown in Fig. 1c. The room temperature Hall measurements reveal an electron carrier concentration of 2 x 10^{19} cm^3 and a Hall mobility of ~4.1 cm^2/V.s. Binding energies of Sc*2p*, Sc*3s*, and Ga*3d* core level photoelectrons and valence band edge were measured using X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS) measurements. These measurements were performed on three different samples: a thick ScN film of 60 nm thickness, a thin ScN film of 3 nm thickness, and a GaN film sample (Fig 1d). The ScN/GaN heterojunction exhibits a straddling type-I bandgap alignment, as shown in Fig. 1e. The valence band offset of $\Delta E_V = 0.77$ eV was measured. Using an ScN energy bandgap of 1.34 eV measured with ARPES and the GaN bandgap of 3.4 eV, the conduction band offset is determined to be $\Delta E_C = 1.29$ eV.

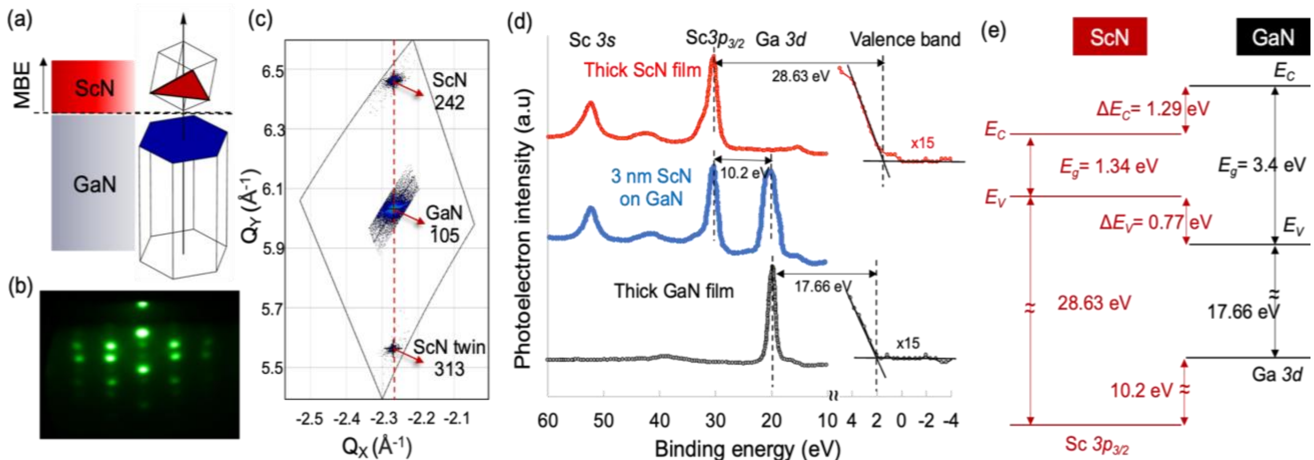

Fig. 1 (a) Schematic of (111) ScN/ (0001) GaN heterostructure, (b) RHEED image of twin cubic ScN film, (c) XRD RSM of ScN and GaN reflections showing in-plane lattice matching, (d) XPS, UPS spectra of thick ScN, ScN/GaN heterojunction and thick GaN film samples (e) Band offset between ScN/GaN heterojunction.