

Band Alignment of ScN/GaN(0001) Heterostructure

H.-W. Shiu (許紘璋)^{1,2}, L.-Y. Chang (張羅嶽)^{1,2}, J.-L. Lou (婁介嶺)^{1,2},
C.-P. Wu (吳佳平)¹, and C.-H. Chen (陳家浩)¹

¹National Synchrotron Radiation Research Center, Hsinchu, Taiwan

²Department of Physics, National Tsing Hua University, Hsinchu, Taiwan

Gallium nitride (GaN) based optoelectronic devices on silicon have attracted a great interest as LEDs and ultraviolet photodetectors [1]. However, the quality of the GaN films was difficult to control and affected the performance of the devices seriously. In order to improve the quality of GaN films on Si, different materials; such as silicon carbide (SiC) or aluminum nitride (AlN) have been used as buffer layer [2]. Recently, an unusual material; namely scandium nitride (ScN), has been found to be a promising buffer layer for growing GaN on Si [3]. ScN is a transition metal nitride semiconductor exhibiting a rock-salt structure with melting point of 2600°C and direct band gap of 2.1-2.4 eV [4]. These properties make it an ideal material to incorporate group-III nitrides with silicon. Accordingly, it is interesting to study the electronic and crystalline structure of this nitride semiconductor and the ScN/Si, ScN/GaN interfacial property, in order to gain insight about this novel material.

We have systematically studied the electronic properties of ScN grown on GaN (0001) surface. The ScN overlayer was grown by the plasma assisted molecular beam epitaxy. An in-situ high resolution X-ray photoemission spectroscopy (HRXPS) measurement was used for the electronic structure and band lineup studies.

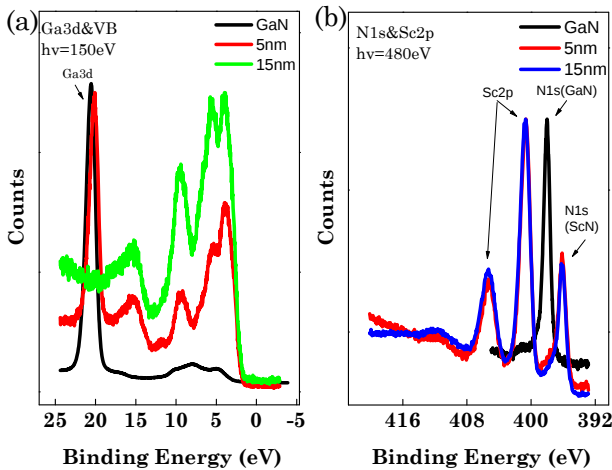


Fig. 1: (a) Ga 3d, valence band (VB), (b) N 1s and Sc 2p spectra of ScN grown on GaN (0001) surface as a function of ScN thickness.

From the set of VB and Ga 3d spectra shown in Fig.

1, it is obviously that the valance band maximum (VBM) and Ga 3d signal shifted with ScN thickness. At lower overlayer thickness, Ga 3d shifted 0.4 eV to lower binding energy compare with bare GaN substrate. This shift is because of the band bending effect when ScN overlayers grown on GaN surface. When ScN film is thick enough (15nm), the pure VBM of ScN could be observed. The binding energy (BE) of these core level lines and VBM were listed in the table shown in Fig. 2.

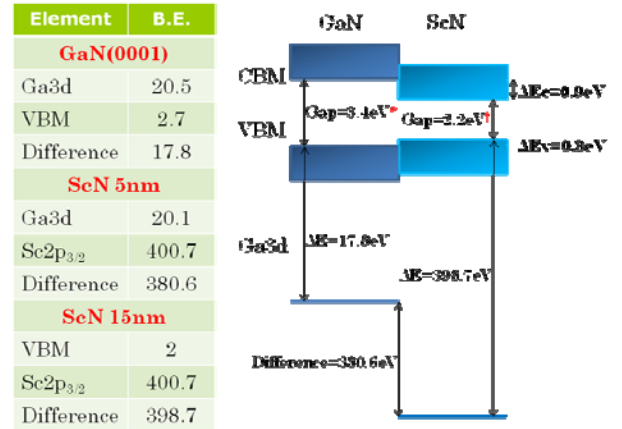


Fig. 2: Schematic diagram of band lineup at ScN/GaN (0001) interface (right hand side) with corresponding core level lines and VBM positions. The gap values of GaN* and ScN* were recorded from ref. [5] and [6], respectively.

The band offset of the ScN/GaN heterostructure was summarized in the diagram shown in Fig.2 (right hand side). A valence band discontinuity of 0.3 eV was found for ScN/GaN. Such that this heterojunction formed straddling type; the discontinuities for valence and conduction bands go into opposite direction.

References

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