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Valence and conduction band alignment at ScN interfaces with 3C-SiC (111) and 2H-GaN (0001)

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In order to understand and predict the behavior of future scandium nitride (ScN) semiconductor heterostructure devices, we have utilized *in situ* x-ray and ultra-violet photoelectron spectroscopy to determine the valence band offset (VBO) present at ScN/3C-SiC (111) and 2H-GaN (0001)/ScN (111) interfaces formed by ammonia gas source molecular beam epitaxy. The ScN/3C-SiC (111) VBO was dependent on the ScN growth temperature and resistivity. VBOs of 0.4 ± 0.1 and 0.1 ± 0.1 eV were, respectively, determined for ScN grown at 925 °C (low resistivity) and 800 °C (high resistivity). Using the band-gaps of 1.6 ± 0.2 and 1.4 ± 0.2 eV previously determined by reflection electron energy loss spectroscopy for the 925 and 800 °C ScN films, the respective conduction band offsets (CBO) for these interfaces were 0.4 ± 0.2 and 0.9 ± 0.2 eV. For a GaN (0001) interface with 925 °C ScN (111), the VBO and CBO were similarly determined to be 0.9 ± 0.1 and 0.9 ± 0.2 eV, respectively. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4894010]

Scandium nitride (ScN) is a transition metal nitride semiconductor that over the past decade has garnered significant interest for nano-electronic,¹ spin-tronic,² opto-electronic,³ electro-acoustic,⁴ and thermo-electric applications.⁵ Despite having a sodium chloride/rock salt crystal structure,⁶ ScN has received the most attention for applications in combination with wurtzite structure wide band gap semiconductors such as silicon carbide (SiC) and gallium nitride (GaN).^{7,8} This is primarily due to the reasonably close lattice matching exhibited between the (111) plane of ScN $(a_0 = 0.3139 \text{ nm})$ and the (111)/(0001) planes of SiC and GaN $(a_0 = 0.3073 \text{ and } 0.3189 \text{ nm}, \text{ respectively}).^{9,10}$ The reported low resistivity¹¹ and band gap of 1.3 ± 0.3 eV (Ref. 12) for ScN, in particular, makes it an interesting material for Ohmic or Schottky contacts to n-type SiC and GaN and also as a conductive substrate or buffer layer for GaN heteroepitaxy on SiC.^{7,13} For these specific applications, the valence and conduction band alignment of ScN to SiC and GaN will play a significant role in charge transport and carrier recombination at these interfaces. In this regard, we have utilized in situ x-ray and UV photoelectron spectroscopy (XPS and UPS) combined with reflection electron energy loss spectroscopy (REELS) to determine the valence and conduction band alignment for interfaces formed by ammonia (NH₃) gas-source molecular beam epitaxy (NH₃-GSMBE) of ScN and GaN on 3C-SiC (111) epilayers on 6H-SiC (0001) substrates.^{14,15}

The ScN and GaN NH₃-GSMBE were performed in a custom built system specifically designed for the heteroepitaxial growth of ScN, GaN, and AlN on SiC substrates. The details of this system and the ScN growth conditions have been previously described.^{16,17} Briefly, source materials in the NH₃-GSMBE system consisted of NH₃ (99.9995%), Sc (99.99%), and Ga (99.99999%). The NH₃ was further purified via an inline metalorganic resin purifier connected directly to a leak valve mounted on the GSMBE chamber. Growth of ScN and GaN were both performed in a back pressure of 10^{-5} – 10^{-4} Torr NH₃ at temperatures of 800–925 °C. The Sc and Ga Knudsen cells were operated at 1300 °C, and 1050 °C, respectively.

The on axis, 6H-SiC (0001) wafers ($N_d \approx 10^{18}/cm^3$) utilized in this study were provided with a 1 μ m 3C-SiC (111) epitaxial layer ($N_d \approx 10^{17}$ /cm³) by Cree, Inc., A 3C-SiC epilayer was selected to minimize possible remnants of the 6H-SiC substrate wafer processing and for consistency with prior investigations of GaN and AlN growth on SiC.¹⁶ The unpolished sides of these wafers were coated with an opaque tungsten film via RF sputtering to increase the thermal heating efficiency of the SiC substrate, as the latter is transparent to the infra-red radiation emitted by the tungsten filament heater. After sputter coating, the wafers were ultrasonicated in trichloroethylene, acetone, and methanol for 10 min each, and then dipped in 10:1 buffered HF for 10 min to remove the 100 nm thermal oxide previously grown on the SiC substrate prior to backside tungsten coating.^{18,19} The wafers were then subsequently degassed/ annealed at 1050 °C in 10⁻⁹Torr vacuum in the GSMBE system for 10-15 min to desorb the remaining monolayer of surface oxide.²⁰ This surface displayed a $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ reconstruction in LEED that has been previously shown to be slightly carbon rich relative to the $(\surd3\times\surd3)R30^\circ$ surface generated by annealing in Si or SiH4. ^{21,22}

The XPS and UPS measurements have been described previously and were performed in a separate vacuum

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chamber attached to the main ultra high vacuum (UHV) transfer line.^{23–25} Briefly, all XPS spectra were collected using Al K α radiation (h ν = 1484.6 eV) in a 2 × 10⁻¹⁰ Torr UHV system equipped with a 100 mm hemispherical electron energy analyzer (VG CLAMII). Conditions previously demonstrated to minimize charging and surface photovoltage effects for GaN/AIN and AIN/6H-SiC (0001) interfaces were utilized.²⁵ Calibration of the binding energy scale for all scans was achieved by periodically taking scans of the Au 4f_{7/2} and Cu 2p_{3/2} peaks from standards and correcting for any discrepancies with the known values (83.98 and 932.67 eV, respectively). A combined Gaussian-Lorentzian curve shape with a linear back-ground was found to best represent the XPS data. UPS measurements were performed with the same energy analyzer and a differentially pumped helium resonance UV lamp.

The method of Kraut,²⁶ previously described in detail,^{23–25} was utilized to determine the valence band offset (VBO) at the ScN/SiC and GaN/ScN interfaces. The method relies on referencing distinct core levels (CLs) in each material to their respective valence band maximum (VBM) and then measuring the relative position of these core levels with respect to one another at their interface. As an example for the ScN/SiC interface, the valence band offset (ΔE_v) was determined according to the following equation:

$$\Delta E_{\rm v}({\rm ScN/SiC}) = ({\rm CL} - {\rm VBM})_{\rm ScN} - ({\rm CL} - {\rm VBM})_{\rm SiC} + \Delta {\rm CL}_{\rm int}, \qquad (1)$$

where (CL - VBM) is the relative position of the core level to the valence band maximum of the bulk material, and ΔCL_{int} is the relative position of the core levels in the two materials at the interface [i.e., $\Delta CL_{int} = (CL_{SiC} - CL_{ScN})_{int}$]. To determine ΔCL_{int} for the ScN/SiC interface, we deposited 2-3 nm of ScN on the 3C-SiC substrate and measured the relative position of the Sc 2p and Si 2p core levels at the interface. For the GaN/SiC interface, 2-3 nm of GaN was deposited on a $\sim 25 \text{ nm}$ thick ScN film previously grown on 3C-SiC, and the relative position of the Ga 3d and Sc 2p core levels were measured. (CL - VBM)_{bulk} is typically measured using thicker films (>20 nm) to minimize or eliminate contributions to the photoemission spectra from the underlying substrate/interface. In our case, we have previously determined (CL - VBM)_{bulk} for the Si 2p core level in 3C-SiC to be 99.3 \pm 0.1 eV,^{24,25} and for the Ga 3d core level in 2H-GaN to be $18.4 \pm 0.1 \text{ eV.}^{27}$

Figure 1 shows an XPS valence band spectrum acquired from a 25 nm thick stoichiometric ScN film heteroepitaxially grown on a 3C-SiC (111)–($\sqrt{3} \times \sqrt{3}$)R30° surface at 800°C. This spectrum is similar to those obtained by Porte for reactive sputtered ScN on a Ta foil²⁸ and Gall for UHV N₂ sputter deposited ScN.¹² The large peak at 29.4 eV is the Sc 3p_{3/2,1/2} core level. This peak is chemically shifted to higher binding energy by 0.5–1 eV relative to the metallic Sc value and is consistent with all Sc being bonded to N.²⁹ No evidence of metallic Sc was observed in the XPS spectra of the Sc 3p_{3/2,1/2} core level or the Sc 2p_{3/2,1/2} as previously noted.¹⁵ The feature at 14.4–19.6 eV is due to primarily N 2s states, and the peak centered roughly at 3.7 eV is the N 2p band.^{12,30} Several prior theoretical calculations have shown



FIG. 1. XPS valence band spectrum for stoichiometric ScN deposited at $800\,^\circ\text{C}$ on 3C-SiC (111).

the upper part of the valence band and valence band maximum for ScN is determined primarily by N 2p related states and the conduction band minimum by Sc 3d states.^{30–32} The O 2p state at 10.4 eV was not detected in the valence band spectrum.¹ However, the O 1s was detected in XPS indicating the presence of ~1%–2% O surface coverage.

To more clearly locate the valence band maximum, a magnification of the upper part of the XPS valence band spectrum is presented in Figure 2 in combination with a higher signal to noise ratio UPS spectrum of the valence band for the same film. A linear extrapolation of the turn in photoemission to the x-axis locates the valence band maximum at $0.7 \pm 0.1 \text{ eV}$ below the system Fermi level in both spectra. Interestingly, the feature at approximately 7.2 eV in the UPS spectrum is noticeably absent from the XPS spectrum. As indicated in a previous publication,¹⁵ the small peak at 7.2 eV could be a possible surface state. As XPS is less surface sensitive relative to UPS, the absence of this feature in the XPS spectrum lends further support to this feature being a surface state. However, additional theoretical investigations of the ScN (111) surface are needed to confirm the exact origin of this feature.

As indicated previously,¹⁵ the Sc $2p_{3/2}$ was well fitted using a mixed Gaussian-Lorentzian curve shape and a linear background (see Figure 3). The peak centroid for the $2p_{3/2}$ core level was determined to be 399.8 ± 0.03 eV and Sc $2p_{3/2}$ -VBM was correspondingly determined to be 399.1 ± 0.1 eV.



FIG. 2. (a) XPS and (b) UPS spectra of the valence band maximum for stoichiometric ScN deposited at 800 °C.



FIG. 3. XPS of Sc 2p3/2,1/2 and N 1s from 200 nm thick ScN on 3C-SiC (111).

For a 2 nm ScN film deposited on the 3C-SiC substrate, the Sc $2p_{3/2}$ and Si 2p core levels were similarly well fitted using single peaks and located at 400.4 eV and 100.7 ± 0.03 eV. Using Sc $2p_{3/2}$ – Si 2p = 299.7 eV and the previously determined values of Si2p-VBM_{SiC} and Sc2p_{3/2}-VBM_{ScN}, we determine the VBO for this ScN/3C-SiC (111) interface to be -0.1 ± 0.1 eV.

We have previously shown that ScN films grown at higher temperatures exhibit increased conductivity/background carrier concentrations, larger band-gaps and a slight (2%-5%) increase in nitrogen content.¹⁵ To examine the influence this may have on the valence band alignment, a second ScN/SiC interface was prepared by growing ScN on 3C-SiC (111) at 925 °C. For this film, a slightly larger value of Sc $2p_{3/2} - VBM = 399.4 \text{ eV}$ was determined. However, the relative position of the Sc $2p_{3/2}$ and Si 2p core levels remained unchanged at 299.7 eV. The resulting VBO is larger at $-0.4 \pm 0.1 \,\text{eV}$ with the increase coming mostly from the increased value of Sc $2p_{3/2}$ – VBM. As discussed previously,¹⁵ the change in Sc $2p_{3/2}$ – VBM with growth temperature and possible stoichiometry is consistent with prior theoretical calculations by Moreno-Armenta that have shown a widening of the ScN band-gap with increasing nitrogen content.³⁰ We have also previously observed similar differences in VBO for GaN/AIN interfaces that corresponded to changes in the GSMBE GaN growth temperature and resulting film properties and XPS CL-VBM.²⁷ Although no sign of chemical intermixing at the ScN/SiC interface was detected in XPS, the slightly different VBO for the two different ScN/SiC interfaces could also be attributed to slight differences in stoichiometry in both the ScN film and at the interface. We have previously shown Sc has a propensity to react with the SiC substrate that is sensitive to temperature,¹⁵ and Guerrero-Sanchez has previously shown Sc prefers substitutional Ga sites on GaN (0001) surfaces.³³

To determine the conduction band offsets (CBO) for the two ScN/SiC (111) interfaces, we utilize the literature value of 2.4 eV for the band-gap of 3C-SiC,²⁴ and the previously determined REELS band-gaps of 1.4 and 1.6 ± 0.2 eV for the 800 and 925 °C ScN films, respectively.¹⁵ The resulting CBOs are 0.9 ± 0.2 and 0.4 ± 0.2 eV for 800 °C and 925 °C ScN interfaces with 3C-SiC (111).

To prepare GaN/ScN interfaces, GaN was grown *in situ* on a 200 nm thick ScN epilayer previously grown at 925 °C on 3C-SiC (111). The GaN was grown at 800 °C using conditions that have been previously shown to produce n-type $(N_d \cong 10^{17}/cm^3)$ GaN films when grown on 6H-SiC using a 20 nm in situ AlN buffer layer.¹⁶ For GaN films grown using these same conditions on 25-200 nm thick ScN (111) films, Raman spectroscopy measurements confirmed the growth of wurtzite structure GaN consistent with prior observations of GaN growth on (111) oriented ScN.^{34,35} Hexagonal (1 \times 1) low energy electron diffraction patterns were also observed in situ post growth further supporting the growth of (0001) oriented GaN on (111) oriented ScN surfaces.^{36,37} Cross section scanning electron microscope images, however, revealed the growth of columnar poly crystalline GaN films consistent with the very broad peaks observed in x-ray diffraction and x-ray rocking curve measurements. Cathodoluminescence measurements of the GaN films grown on ScN also showed broad and weak intensity donor bound exciton peaks. Although the electrical properties of the GaN on ScN films were not characterized in detail, they exhibited similar resistivities to the previously mentioned GaN films grown on AlN/6H-SiC.16

To determine the band alignment at GaN (0001)/ScN (111) interfaces, 2 nm of GaN was deposited on a 200 nm thick, 925 °C ScN film and XPS was used to measure the relative position of the Ga 3d and Sc $2p_{3/2}$ core levels at the interface. The value of Sc $2p_{3/2}$ – Ga 3d was determined to be 380.2 ± 0.03 eV. For a thicker 100 nm GaN film grown on the same ScN film, the position of the Ga 3d core level relative to the GaN VBM was confirmed to be 18.4 ± 0.1 eV in agreement with previous results for GaN grown on AlN and SiC under identical conditions. Using these values and the literature value of 3.4 eV for the band-gap of GaN,²⁴ the VBO and CBO for the GaN (0001)/ScN (111) interface were determined to be 0.9 ± 0.1 and 0.9 ± 0.2 eV, respectively.

The authors are unaware of any prior measurements of the band alignment between ScN and other materials. We do note that Perjeru *et al.*³⁸ has previously measured the electrical rectifying characteristics of n-ScN/n-GaN heterojunctions and observed turn-on voltages of 1.26-1.56 V with a built in potential of 1 V. This value is in reasonable agreement with the CBO of 0.9 ± 0.2 eV determined here for the n-GaN (0001)/n-ScN (111) interface. Our results are also consistent with current-voltage measurements by Kaplan that determined a barrier height of 1 eV for a Sc/ScN/GaN heterostructure.⁹

A consistency check on the GaN (0001)/ScN (111) and ScN/SiC (111) VBOs can also be performed using the rules of transitivity and commutativity^{39,40} and previously reported values for the VBO at GaN (0001)/3C-SiC (111) interfaces.²⁴ The transitivity and commutativity rules for VBOs, respectively, state that

$$\Delta E_{\rm v}(1/2) + \Delta E_{\rm v}(2/3) + \Delta E_{\rm v}(3/1) = 0, \qquad (2)$$

$$\Delta E_{\rm v}(2/3) = \Delta E_{\rm v}(3/2),\tag{3}$$

where 1/2 signifies the GaN/SiC interface in question, 2/3 signifies the SiC/ScN interface, and 3/1 signifies the ScN/GaN interface. Using the above rules and the GaN/ScN and ScN/SiC VBO data for 925 °C ScN, we deduce a GaN/SiC VBO of 0.5 eV which is in excellent agreement with the



FIG. 4. Schematic flat band diagram showing the VBO and CBO for $925 \,^{\circ}$ C ScN with 3C-SiC (111) and 2H-GaN (0001).

value of $0.5 \pm 0.1 \text{ eV}$ previously experimentally determined for the GaN (0001)/3C-SiC (111) interface.²⁴

In summary, we have utilized XPS and UPS to investigate the VBO present at interfaces between ScN and 2H-GaN and 3C-SiC (see Figure 4). The conduction band alignment was further deduced using the measured VBOs and the band-gap for ScN determined by prior REELS measurements. For high resistivity ScN grown at 800 °C on 3C-SiC (111), a type I interfacial band alignment was determined with VBO and CBO of -0.1 ± 0.1 and 0.9 ± 0.2 eV, respectively. For low resistivity ScN grown at 925 °C on 3C-SiC (111), a type I interfacial band alignment was also determined with VBO and CBO of -0.4 ± 0.1 and 0.4 ± 0.2 eV, respectively. For the GaN (0001)/ScN (111) interface, a type I band alignment was also deduced with VBO and CBO of 0.9 ± 0.1 and 0.9 ± 0.2 eV, respectively.

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- ¹J. Dismukes, W. Yim, and V. Ban, J. Cryst. Growth 13/14, 365 (1972).
- ²A. Herwadkar, W. Lambrecht, and M. van Schilfgaarde, Phys. Rev. B 77, 134433 (2008).
- ³C. Constantin, H. Al-Brithen, M. Haider, D. Ingram, and A. Smith, Phys. Rev. B **70**, 193309 (2004).
- ⁴R. Matloub, H. Hadad, A. Mazzalai, N. Chidambaram, G. Moulard, C. Sandu, Th. Metzger, and P. Muralt, Appl. Phys. Lett. **102**, 152903 (2013).
- ⁵B. Saha, T. Sands, and U. Waghmare, J. Appl. Phys. 109, 83717 (2011).
- ⁶Z. Gu, J. Edgar, J. Pomeroy, M. Kuball, and D. Coffey, J. Mater. Sci. **15**, 555 (2004).
- ⁷J. Edgar, T. Bohnen, and P. Hageman, J. Cryst. Growth **310**, 1075 (2008).
- ⁸M. Ortiz-Libreros, F. Perjeru, X. Bai, and M. Kordesch, Appl. Surf. Sci. **175–176**, 512 (2001).
- ⁹R. Kaplan, S. Prokes, S. Binari, and G. Kelner, Appl. Phys. Lett. **68**, 3248 (1996).

- ¹⁰H. Morkoc, S. Strite, G. Gao, M. Lin, B. Sverdlov, and M. Burns, J. Appl. Phys. **76**, 1363 (1994).
- ¹¹P. Burmistrova, J. Maassen, T. Favaloro, B. Saha, S. Salamat, Y. Koh, M. Lundstrom, A. Shakouri, and T. Sands, J. Appl. Phys. **113**, 153704 (2013).
- ¹²D. Gall, M. Stadele, K. Jarrendahl, I. Petrov, P. Desjardins, R. Haasch, T. Lee, and J. Greene, Phys. Rev. B 63, 125119 (2001).
- ¹³H. Al-Brithen and A. Smith, Appl. Phys. Lett. 77, 2485 (2000).
- ¹⁴S. King, "Surface and interface characterization of SiC and III-V nitrides," Ph.D. dissertation (North Carolina State University, Raleigh, 1997).
- ¹⁵S. King, R. Nemanich, and R. Davis, "Gas source molecular beam epitaxy of scandium nitride on silicon carbide and gallium nitride surfaces," J. Vac. Sci. Technol. A (to be published).
- ¹⁶S. King, E. Carlson, R. Therrien, J. Christman, R. Nemanich, and R. Davis, J. Appl. Phys. 86, 5584 (1999).
- ¹⁷S. King, M. Benjamin, R. Nemanich, R. Davis, and W. Lambrecht, in *Gallium Nitride and Related Materials: The First International Symposium*, edited by R. D. Dupuis, J. A. Edmond, S. Nakamura, and F. A. Ponce (Mater. Res. Soc. Symp. Proc., 1996), Vol. 395, p. 375.
- ¹⁸S. King, R. Nemanich, and R. Davis, J. Electrochem. Soc. **146**, 1910 (1999).
- ¹⁹S. King, R. Nemanich, and R. Davis, J. Electrochem. Soc. **146**, 2648 (1999).
- ²⁰S. King, R. Nemanich, and R. Davis, J. Electrochem. Soc. **146**, 3448 (1999).
- ²¹S. King, R. Davis, and R. Nemanich, Surf. Sci. 603, 3104 (2009).
- ²²S. King, C. Ronning, R. Davis, R. Busby, and R. Nemanich, J. Appl. Phys. 84, 6042 (1998).
- ²³S. King, L. Smith, J. Barnak, J. Ku, J. Christman, M. Benjamin, M. Bremser, R. Nemanich, and R. Davis, in *Gallium Nitride and Related Materials: The First International Symposium*, edited by R. D. Dupuis, J. A. Edmond, S. Nakamura, and F. A. Ponce (Mater. Res. Soc. Symp. Proc., 1996), Vol. 395, p. 739.
- ²⁴S. King, R. Davis, C. Ronning, and R. Nemanich, J. Electron. Mater. 28, L34 (1999).
- ²⁵S. King, R. Davis, C. Ronning, M. Benjamin, and R. Nemanich, J. Appl. Phys. 86, 4483 (1999).
- ²⁶E. Kraut, R. Grant, J. Waldrop, and S. Kowalczyk, Phys. Rev. Lett. 44, 1620 (1980).
- ²⁷S. King, C. Ronning, R. Davis, M. Benjamin, and R. Nemanich, J. Appl. Phys. 84, 2086 (1998).
- ²⁸L. Porte, J. Phys. C: Solid State Phys. **18**, 6701 (1985).
- ²⁹J. Gimzewski, D. Fabian, L. Watson, and S. Affrossman, J. Phys. F: Met. Phys. 7, L305 (1977).
- ³⁰M. Moreno-Armenta and G. Soto, Comput. Mater. Sci. 40, 275 (2007).
- ³¹N. Takeuchi and S. Ulloa, Phys. Rev. B **65**, 235307 (2002).
- ³²C. Stampfl, W. Mannstadt, R. Asahi, and A. Freeman, Phys. Rev. B 63, 155106 (2001).
- ³³J. Guerrero-Sanchez, F. Sanchez-Ochoa, G. Cocoletzi, J. Rivas-Silva, and N. Takeuchi, Thin Solid Films **548**, 317 (2013).
- ³⁴M. Moram, M. Kappers, Z. Barber, and C. Humphreys, J. Cryst. Growth 298, 268 (2007).
- ³⁵M. Moram, Y. Zhang, M. Kappers, Z. Barber, and C. Humphreys, Appl. Phys. Lett. **91**, 152101 (2007).
- ³⁶M. Moram, M. Kappers, T. Joyce, P. Chalker, Z. Barber, and C. Humphreys, J. Cryst. Growth 308, 302 (2007).
- ³⁷J. Hall, M. Moram, A. Sanchez, S. Novikov, A. Kent, C. Foxon, C. Humphreys, and R. Campion, J. Cryst. Growth **311**, 2054 (2009).
- ³⁸F. Perjeru, X. Bai, M. Ortiz-Libreros, R. Higgins, and M. Kordesch, Appl. Surf. Sci. 175–176, 490 (2001).
- ³⁹A. Katnani and R. Bauer, Phys. Rev. B **33**, 1106 (1986).
- ⁴⁰S. King, M. Paquette, J. Otto, A. Caruso, J. Brockman, J. Bielefeld, M. French, M. Kuhn, and B. French, Appl. Phys. Lett. **104**, 102901 (2014).