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## Dependence of (0001) GaN/AIN valence band discontinuity on growth temperature and surface reconstruction

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X ray and ultraviolet photoelectron spectroscopies have been used to determine the heterojunction valence band discontinuity at the (0001) GaN/AlN interface. Type I discontinuity values of  $0.5\pm0.2$  eV were determined for GaN grown on AlN at 650 °C and  $0.8\pm0.2$  eV for GaN grown on AlN at 800 °C. These values are critically evaluated with respect to film quality, the results of other experimental studies, and theory. © *1998 American Institute of Physics*. [S0021-8979(98)01716-2]

#### I. INTRODUCTION

The compound semiconductors GaN and AlN are completely miscible with band gaps of 3.40 and 6.2 eV, respectively. Applications based on heterostructures and band-gap engineering of these two materials and their alloys have been realized including UV/visible optoelectronics and highfrequency devices.<sup>1-3</sup> Charge transport and quantum confinement can affect these devices.<sup>4</sup> Reliable knowledge of the valence band discontinuity ( $\Delta E_V$ ) for the GaN/AlN interface is extremely important to the advancement of III-V nitride technology. Accordingly, several authors using a variety of characterization techniques have reported  $\Delta E_V$  values for GaN/AlN heterojunctions fabricated by different growth techniques including electron cyclotron resonance- molecular beam epitaxy (MBE),<sup>5–7</sup> NH<sub>3</sub>-gas source (GSMBE),<sup>8</sup> and organometallic vapor phase epitaxy (OMVPE)9,10 on  $Al_2O_3$ , 9,10 and  $6H-SiC^{5-8}$  substrates. Unfortunately, the electrical, optical, and microstructural characteristics of these materials and the associated interfaces prepared and deposited by the various techniques are quite different, and the corresponding values reported for the  $\Delta E_V$  range from 0.5 eV (Ref. 9) to 1.4 eV (Refs. 7 and 8) (see Table I, which also includes values from theory).<sup>11-14</sup> In a separate paper,<sup>15</sup> we have shown that for GaN grown via NH3-gas source MBE on a high temperature monocrystalline AlN buffer layer, a 3D-2D growth transition can be observed with a corresponding change in the electrical, optical, and microstructural properties of the resulting GaN films. In this paper, we show that the valence band discontinuity for the (0001) GaN/ AlN interface also changes with this transition.

#### **II. EXPERIMENT**

A GSMBE with a base pressure of  $3 \times 10^{-10}$  Torr was designed and constructed specifically for the growth of III–V nitride thin films.<sup>16</sup> Source materials in the system included

Al (99.9999%), Ga (99.99999%), and NH<sub>3</sub> (99.9995%). The Al and Ga were evaporated from 25 cc "cold lip" and dual filament Knudsen cells, respectively.

The substrates used in this study were  $1.5 \times 1.5$  cm<sup>2</sup> pieces cut out of off-axis [4° toward (1120)] *n*-type ( $N_d$ = $10^{18}/\text{cm}^3$ ) 6H–SiC (0001)<sub>Si</sub> wafers. All samples were received with an  $\approx 1 \ \mu m$  *n*-type epitaxial layer ( $N_d = 5$  $\times 10^{17}$  cm<sup>3</sup>). They were ultrasonically and sequentially rinsed in trichloroethylene, acetone, and methanol, dipped in 10:1 buffered HF for 10 min and mounted to a Mo sample holder. The *in situ* procedure used for the final cleaning step of the 6H-SiC substrates was similar to that described by Kaplan and Kern.<sup>17,18</sup> Briefly, each SiC wafer was annealed in the GSMBE system in a flux of  $10^{-6} - 10^{-5}$  Torr SiH<sub>4</sub> for 15-20 min at 950-1050 °C. Analysis via Auger electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS) revealed oxygen-free, silicon terminated SiC surfaces which displayed  $(1 \times 1)$  low energy electron diffraction (LEED) patterns.

An approximately 250 Å single crystalline AlN film grown at 1050 °C in  $\approx 10^{-5}$  Torr NH<sub>3</sub> on each (0001)<sub>Si</sub> 6H–SiC sample was used as a buffer layer for the growth of GaN. Each AlN film displayed a (2×2) reconstructed surface in LEED immediately after growth. To achieve the growth of the GaN films on the AlN buffer layers, the latter was heated to 650–800 °C in  $10^{-4}$  Torr ( $\approx$ 50 sccm) ammonia, after which the Ga cell was opened. After the desired GaN thickness had been achieved, the Ga cell was closed and the GaN film allowed to cool in ammonia to approximately 600 °C after which the ammonia valve was closed. Films grown at 650 °C had a (1×1) reconstructed surface; whereas, films grown at 800 °C displayed (2×2) reconstructed surfaces in LEED.

After growth, the films were transformed *in situ* for analysis, and the XPS and ultraviolet photoelectron spectroscopy (UPS) experiments were performed in an UHV chamber (base pressure= $2 \times 10^{-10}$  Torr) equipped with a dual anode (Mg/Al) x-ray source, a differentially pumped helium

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TABLE I. Published data for the valence band discontinuity GaN/AlN  $\Delta E_V$ . (PL/CL=photoluminescence/ cathodoluminescence, LMTO=linear muffin tin orbital, LAPW=linearized augmented plane wave, PWP =plane-wave pseudopotential).

$\Delta E_V$ GaN/AlN	Orientation	Relax/Strain	Technique	Author
0.8±0.3 eV	(0001)		XPS	Martin et al. (Ref. 5)
0.7±0.24 eV	(0001)		XPS	Martin et al. (Ref. 6)
0.5 eV	(0001)		PL metal imp.	Baur et al. (Refs. 9, 10)
1.36±0.07 eV	(0001)		XPS	Waldrop and Grant (Ref. 8)
1.4 eV	(0001)		CL/PL	Sitar et al. (Ref. 7)
0.85 eV	(110)	4.435 Å	LMTO	Albensi et al. (Ref. 12)
0.75 eV	(001)	4.435 Å	LMTO	Ke et al. (Ref. 14)
0.77 eV	(111)	4.435 Å	LMTO	Ke et al. (Ref. 14)
0.81 eV	(110)	4.435 Å	LMTO	Ke et al. (Ref. 14)
0.83 eV	(0001)	3.11 Å	LMTO	Ke et al. (Ref. 14)
0.84±0.1 eV	(001)	4.435 Å	LAPW	Wei et al. (Ref. 11)
0.81±0.1 eV	(0001)	3.15 Å	LAPW	Wie et al. (Ref. 11)
0.73 eV	(0001)	3.11 Å	PWP	Nardelli et al. (Ref. 13)
0.58 eV	(0001)	3.15 Å	PWP	Nardelli et al. (Ref. 13)
0.44 eV	(0001)	3.19 Å	PWP	Nardelli et al. (Ref. 13)

resonance UV lamp, and a 100 mm hemispherical electron energy analyzer (VG CLAM II). All XPS spectra were obtained using Mg  $K\alpha$  radiation ( $h\nu$ = 1253.6 eV). Calibration of the binding energy scale for all scans was achieved by periodically measuring the positions of the Au 4 $f_{7/2}$  and Cu  $2p_{3/2}$  peaks from clean standard samples and correcting them to 83.98 and 932.67 eV, respectively. A combination Gaussian–Lorentzian curve shape with an "s-shape" background best represented the XPS data. All UPS spectra were acquired using the unmonochromated He I line ( $h\nu$ = 21.2 eV) from the UV lamp. The LEED patterns were obtained using an 80 eV, 1 mA beam.

The method used for calculating the GaN/AlN valence band discontinuity was similar to that of Waldrop and Grant<sup>8</sup> and Kraut et al.<sup>19</sup> The basic scheme of this approach is to reference the valence band maximum energy to a core level energy from each semiconductor and then use the measured difference between the two core level energies from a junction between the two semiconductors to indirectly determine the discontinuity. Specifically, the position of one core level (CL) from the substrate (AlN) is measured with respect to the substrate valence band maximum (VBM), i.e., (VBM-CL)<sup>AlN</sup><sub>bulk</sub>. Subsequently, a thin layer ( $\approx$ 15–20 Å) of the second semiconductor (GaN) is deposited on the substrate and the difference between the substrate and film core levels are measured, i.e., (CL<sup>AIN</sup>-CL<sup>GaN</sup>)<sub>interface</sub>. Finally, the thickness of the overlying film is increased beyond the sampling depth of XPS (≈250 Å) and the CL-to-VBM energy is measured for the film, i.e., (VBM-CL)<sup>GaN</sup><sub>bulk</sub>. The valence band discontinuity between the two semiconductors is then given as:

$$-\Delta E_V(\text{GaN/AlN}) = (\text{VBM-CL})_{\text{bulk}}^{\text{AlN}} - (\text{VBM-CL})_{\text{bulk}}^{\text{GaN}} + (\text{CL}^{\text{AlN}} - \text{CL}^{\text{GaN}})_{\text{int}}.$$
 (1)

Waldrop and Grant<sup>8</sup> and Martin *et al.*<sup>5,6</sup> used XPS to determine the core level and valence band maxima energies. In contrast, we used both XPS and UPS to determine the VBM of AlN and GaN. The core level energies were measured via XPS.

#### **III. RESULTS AND DISCUSSION**

The measurements of the AlN VBM position were complicated by the presence of significant amounts of emission from He  $I_{\beta}$  radiation in the UPS spectra, as shown in Fig. 1(a). The effects of sample charging were excluded from the spectra; however, a sharp band edge was not observed. This was due to the low quality of the AlN and the significant number of surface defects which also created levels in the band tails. The location of the VBM in the UPS VB spectra was determined by extrapolating a straight line through the leading edge of the spectra to the energy axis. A value of 71.5±0.1 eV was determined for Al 2p-VBM<sub>AIN</sub> using this analysis procedure for several AlN films with a (2×2) reconstructed surface. A slightly lower value of 71.3±0.3 eV



FIG. 1. (a) UPS and (b) XPS valence band spectra of  $(2\times2)$  (0001) AlN grown by GSMBE.



FIG. 2. (a) UPS valence band spectra of  $(2\times2)$  (0001) GaN grown by GSMBE at 800 °C as well as (b) UPS and (c) XPS valence band spectra of  $(1\times1)$  (0001) GaN grown at 650 °C.

was determined from the XPS spectra, as shown in Fig. 1(b). The intermediate value of  $71.4\pm0.2$  eV for Al 2p-VBM<sub>AlN</sub> was chosen for the further calculations.

Determination of the VBM for GaN was straightforward, as no charging of the samples occurred and the films were of a much higher quality. Extrapolation of the leading edge of the UPS VB spectra for GaN grown at 800 °C [(2×2) reconstruction] to the energy axis yielded a value of  $2.4\pm0.1$  eV, as shown in Fig. 2(a), which is in excellent agreement with the  $2.4\pm0.2$  eV value obtained from the XPS VB spectra (data not shown). Comparison of the UPS and the XPS VB spectra from 650 to 800 °C GaN revealed that the position of the GaN VBM moved only 0.2 eV closer to the Fermi level when the growth temperature was increased from 650 to 800 °C [Figs. 2(b) and 2(c)]. A larger shift was observed in the positions of the GaN core levels, which resulted in a 0.6–0.7 eV change in the CL–VBM<sub>GaN</sub> value with growth temperature and reconstructed surface (see Fig. 3).

The positions of the Al 2*p*, N 1*s*, and Ga 3*p*, 3*d*, and 2*p* core levels were recorded as a function of thickness of GaN grown on AlN. These data revealed that the values for  $CL_{GaN}-CL_{AlN}$  were similar to within  $\pm 0.2$  eV regardless of film thickness. However, for purposes of comparison, values of  $\Delta E_V$  were calculated using  $AlN_{CL}-GaN_{Cl}$  data taken at film thicknesses in the range of 18–22 Å. As noted by Waldrop and Grant,<sup>8</sup> this thickness is beyond the reported critical



FIG. 3. XPS core level spectra of (top) AlN (2×2), (middle) GaN (1×1) grown at 650 °C and (bottom) GaN (2×2) grown at 800 °C. Dots are the measured data and solid lines represent fits.

thickness for GaN on AlN<sup>20</sup> and should minimize strain effects.

We have summarized the measured XPS core level spectra in Fig. 3. A satisfying agreement between the measured and the fitted spectra could be achieved using only one component for all core level lines, as is shown by the lines in Fig. 3. The shift in the positions of the GaN Ga 3d and N 1s core levels is clearly visible. The full width at half-maximum (FWHM) of 1.45 eV did not change in the Ga 3d core level as a function of the growth temperature, however, the N 1s line is sharper (FWHM=1.16 eV) for the GaN grown at 800 °C compared to the GaN grown at 650 °C (FWHM = 1.34 eV).

Values for the GaN/AlN valence band discontinuity for GaN on AlN were calculated using Eq. (1). For GaN grown at 800 °C on AlN,  $\Delta E_V$  (GaN/AlN)=0.8±0.2 eV; for GaN grown at 650 °C,  $\Delta E_V$ =0.5±0.2 eV.

Two reports of the (0001) GaN/AlN band alignment based on XPS measurements have been previously published by Martin *et al.*<sup>5,6</sup> and Waldrop and Grant.<sup>8</sup> Both groups proposed a type I band alignment between GaN and AlN but with the significantly different valence band discontinuities of  $0.8\pm0.3 \text{ eV}^{5,6}$  and  $1.36\pm0.07 \text{ eV}.^8$  Similar values for  $\text{CL}_{\text{AlN}}$ - $\text{CL}_{\text{GaN}}$  were measured in these and the present studies; thus, most of the discrepancy in  $\Delta E_V$  arises from the values determined for CL–VBM<sub>AlN</sub> and CL–VBM<sub>GaN</sub>. Table II summarizes the Al 2p–VBM<sub>AlN</sub> and Ga  $3d_{\text{CL}}$ -VBM<sub>GaN</sub> data. Values from other studies are also included.<sup>21–25</sup>

The data in Table II show a large distribution. It is interesting to note that the lowest values for Ga 3d-VBM<sub>GaN</sub> were all obtained from films/surfaces derived from exposure

TABLE II. CL-VBM data for AlN and GaN reported by various investigators.

Author	Al $2p - VBM_{AIN}$	Ga $3d - VBM_{GaN}$	Al $2p$ -Ga $3d$
Bermudez et al. (Ref. 21)	71.9±0.2 eV	18.4±0.2 eV	
This work	71.4±0.2 eV	17.9±0.1 eV (650 °C)	54.0±0.1 eV
		18.4±0.1 eV (800 °C)	53.8±0.1 eV
Bermudez et al. (Ref. 22)		17.9±0.2 eV	
Waldrop and Grant (Ref. 8)	70.6±0.07 eV	17.76±0.07 eV	54.2±0.05 eV
Martin et al. (Ref. 5)	70.6±0.3 eV	17.1±0.3 eV	
Matrin et al. (Ref. 6)	70.44±0.04 eV 17.02±0.09 eV		
Hunt et al. (Ref. 23)		17.2 eV	
Ma et al. (Ref. 24)		17.1 eV	
Dhesi et al. (Ref. 25)		18.2 eV	

to high energy ions of Ar, Xe, or N. In the case of Hunt et al.,<sup>23</sup> the CVD GaN surfaces examined were prepared by sputtering with Xe, Ar, or N ions. They observed significant depletion of nitrogen from the surface for Xe and Ar sputtering. In the case of N sputtering, the surface was observed to loose nitrogen initially but increase in stoichiometry with time. All surfaces were structurally highly disordered after sputtering and required annealing at 500 °C to display a reflection high energy electron diffraction (RHEED) pattern. In the case of Ma et al.,<sup>24</sup> it was observed that extended Ar sputtering produced essentially metallic Ga 3d features and the appearance of photoemission leading out to the Fermi level. It is well documented that GaN films prepared by ECR-GSMBE are composed of a variety of different defects and that exposure to this nitrogen source could also induce surface disorder and defects.

We note that our value for Ga 3d-VBM for GaN grown at 650 °C is in close agreement with that obtained by Grant and Waldrop<sup>8</sup> for films grown under similar conditions. Our films grown at 650 °C were highly conductive with carrier concentrations of  $>10^{20}$  cm<sup>-3</sup>. Owing to the low growth temperature and previous calculations, it seems reasonable to suggest that the high carrier concentration is due to the formation of a large number of nitrogen vacancies produced due to insufficient decomposition of the NH<sub>3</sub>. This is supported by the fact that for 800 °C GaN growth, we observed that the carrier concentration decreased significantly down to  $10^{16}-10^{17}$  cm<sup>-3</sup>. Correspondingly, Ga 3*d*-VBM was observed to increase to 18.4 eV. This value is supported by the results of Dhesi *et al.*<sup>25</sup> They found Ga 3d-VBM<sub>GaN</sub>=18.2 eV for "high quality" ECR-GSMBE films cleaned by a combined Ga  $flux/N_2^+$  ion sputter clean. Thus, these data strongly suggest that Ga 3d-VBM is extremely sensitive to surface stoichiometry or surface defects. Although the data for Al 2p-VBM<sub>AlN</sub> in Table II is not as extensive, we assert that similar arguments can be made for AlN surfaces.

As the AlN and GaN CL-VBM values are sensitive to the location of the VBM, an alternative explanation for the observed discrepancy is that the differences are a result of the different methods used to locate the VBM. The energy position of the VBM for AlN and GaN was determined in this study and those reported in Refs. 21–25 by a straightline extrapolation of the leading edge of the XPS/UPS valence band spectra to the energy axis. If a significant number of occupied states in the band gap of AlN or GaN exist at the surface, photoemission could occur from these states and would cause the valence band to falsely appear closer to the Fermi level. This would result in larger values for Al  $2p-VBM_{AlN}$  and Ga  $3d-VBM_{GaN}$ . In fact owing to this effect, Bermudez has recently changed his originally reported value of 18.4 eV (Ref. 21) for Ga 3d-VBM<sub>GaN</sub> to 17.9 eV.<sup>22</sup> This effect could also explain why our CL-VBM values are much larger than those reported by Martin et al.<sup>5,6</sup> and Waldrop and Grant.<sup>8</sup> Their XPS VB spectra were fitted to calculated VBDOS (VB density of states). In this case, the effect of surface states on the location of the VBM is excluded. For GaN films grown in the present research at 650 °C (i.e., conditions identical to Waldrop and Gant<sup>8</sup>) a value of  $17.9\pm0.1$  eV was obtained for Ga 3d-VBM<sub>GaN</sub> which is in good agreement with their value. For 800 °C grown GaN, we note that Dhesi et al.<sup>25</sup> obtained a similar value for Ga 3d-VBM<sub>GaN</sub>. Their detailed angle resolved photoemission study indicated the existence of a surface state, but this state was located below the VBM and hence did not effect the location of the VBM via a straight line extrapolation. All of the above indicate that photoemission from surface states as well as the method used to determine the VBM are not the source of the discrepancy among the various measurements.

A third explanation for the differences in CL-VBM values could be attributed to photovoltage effects. Our data and those of others show the VBM of clean GaN surfaces be located only 2.4-2.7 eV below the Fermi level. For the doping levels in these films, the VBM should be located  $\approx 3.3$ eV below the Fermi level given that  $E_g = 3.39$  eV. This indicates the existence of  $\approx 1 \text{ eV}$  upward band bending at the GaN surface. This could be explained by the presence of surface states in sufficiently small densities as to be undetected in photoemission but in sufficient quantity to still pin the Fermi level in the gap and create band bending at the surface. This seems likely as Bermudez et al.<sup>21,22</sup> have demonstrated that the GaN VBM can be relaxed back to 3.4 eV below  $E_F$ by exposure to  $XeF_2$  and partially relaxed by exposure to  $O_2$ . The presence of band bending at the surfaces of wide bandgap semiconductors could result in photovoltage effects which could also account for the observed discrepancies in the CL-VBM data. As we used two photon sources (i.e., different photocurrents) to measure the CLs and VBMs, this may explain the difference between our value of  $17.9\pm0.1$ 

eV for Ga 3d–VBM<sub>GaN</sub> from (1×1) unreconstructed GaN films grown at 650 °C and our value of 18.4 eV from (2×2) reconstructed GaN films grown at 800 °C. However, the fact that the VBM for GaN was observed at the same energy position in both XPS and UPS strongly indicates the lack of any photovoltage effects. Finally, in a previous study, Bermudez<sup>21,22</sup> was able to induce at most a 0.2 eV change in VBM with a Hg lamp due to photovoltaic effects. This shift is not large enough to explain the effects observed in this study.

We conclude that the range of CL-VBM values reported for GaN and AlN are not a result of measurement artifacts due to the existence of surface states and/or photovoltaic effects. The most plausible explanation appears to be attributed in differences in film/surface preparation, defects, strain, and stoichiometry of the GaN and AlN films. The electrical, optical, and microstructural properties of GaN films grown in this study by the NH<sub>3</sub> GSMBE technique at temperatures of 650 and 800 °C are different. We observed<sup>15</sup> that GaN growth at 650 °C occurred via a 2D/Stranski-Krastanov growth mechanism with the corresponding films exhibiting rough surfaces, extremely high carrier concentrations  $(N_d$  $=10^{19-20}$  cm<sup>-3</sup>), and broad, weak photoluminescence (PL) spectra. In contrast, GaN growth at 800 °C occurred via a two-dimensional/Frank van der Merwe growth mechanism with the corresponding films exhibiting smooth surfaces. Lower carrier concentrations ( $N_d = 10^{16} \text{ cm}^{-3}$ ) and sharp PL were also measured. The defect levels in these films and at the interfaces are significantly different and lead to the increase in  $\Delta E_V$  from 0.5 to 0.8 eV with the increase in growth temperature.

The value of 0.8 eV obtained for 800 °C GaN on AlN is in excellent agreement with all of the reported theoretical values for  $\Delta E_V$  GaN/AlN in which GaN is strained to the lattice constant of AlN at the interface. In addition, the value of 0.5 eV for 650 °C GaN/AlN is also in agreement with values of 0.44 and 0.48 eV predicted by Nardelli *et al.*<sup>13</sup> and Ke *et al.*<sup>14</sup> for  $\Delta E_V$  for a GaN/AlN interface in which the GaN is allowed to adopt its bulk lattice constant/structure. This makes sense as our GaN films grew in a threedimensional manner at 650 °C and were free to grow in a relaxed manner. The growth occurred via a two-dimensional/ Frank van der Merwe growth mechanism for our GaN films at 800 °C and hence the GaN/interface grew strained to the AlN lattice.

#### **IV. CONCLUSION**

XPS and UPS were used to determine the heterojunction valence band discontinuity for the (0001) GaN/AlN inter-

face. For GaN growth on AlN at 650 °C, a type I valence band discontinuity of  $0.5\pm0.2$  eV was determined; a type I discontinuity of  $0.8\pm0.2$  eV was determined for GaN grown on AlN at 800 °C.

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