

Band offset measurements of the $\text{Si}_3\text{N}_4/\text{GaN}$ (0001) interface

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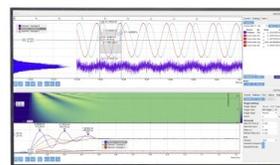
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Band offset measurements of the Si₃N₄/GaN (0001) interface

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X-ray photoelectron spectroscopy and ultraviolet photoelectron spectroscopy were used to measure electronic states as Si₃N₄ was deposited on clean GaN (0001) surfaces. The *n*-type (2×10^{18}) and *p*-type (1×10^{17}) GaN surfaces were atomically cleaned in NH₃ at 860 °C, and the *n*- and *p*-type surfaces showed upward band bending of $\sim 0.2 \pm 0.1$ eV and downward band bending of 1.1 ± 0.1 eV, respectively, both with an electron affinity of 3.1 ± 0.1 eV. Layers of Si (~ 0.2 nm) were deposited on the clean GaN and nitrided using an electron cyclotron resonance N₂ plasma at 300 °C and subsequently annealed at 650 °C for densification into a Si₃N₄ film. Surface analysis was performed after each step in the process, and yielded a valence band offset of 0.5 ± 0.1 eV. Both interfaces exhibited type II band alignment where the valence band maximum of GaN lies below that of the Si₃N₄ valence band. The conduction band offset was deduced to be 2.4 ± 0.1 eV, and a change of the interface dipole of 1.1 ± 0.1 eV was observed for Si₃N₄/GaN interface formation. © 2003 American Institute of Physics. [DOI: 10.1063/1.1601314]

I. INTRODUCTION

Gallium nitride has been established as a material of choice for high frequency electronic and optoelectronic applications. In the fabrication of devices based on heterostructures, the interfacial band alignment is of significant interest. Investigation of heterojunction band discontinuities is important for device design because the valence and conduction band offsets determine the transport and confinement properties at the interface. A fundamental objective for technology and basic research would be the control of the band discontinuities.¹ The use of Si₃N₄ as a passivation layer on GaN-based high voltage devices and as a gate insulator in field effect transistor (FET) devices are potential applications that require knowledge of the band alignment of this interface.

Recent studies of the electrical properties of the Si₃N₄/GaN interface by Arulkumaran *et al.*² and Nakasaki *et al.*³ have reported interface trap densities of 6.5×10^{11} and 5.0×10^{11} eV⁻¹ cm⁻² with clear deep depletion behavior. Chang *et al.*⁴ found that silicon nitride passivation enhances light output and increases the reliability of GaN-based light emitting diodes by reducing the leakage current. Electrical data in the literature indicate the promise of advanced GaN metal-insulator-semiconductor (MIS) devices.²⁻⁴ While several groups have employed photoemission techniques to study GaN/metal interfaces,⁵⁻⁷ only Nakasaki *et al.*³ report band offsets for GaN/Si₃N₄ interfaces. They report type I band alignment with a valence band offset of 1.0–1.2 eV for the Si₃N₄/GaN(0001) interface.

Application of the electron affinity model (EAM) is an initial approach to characterizing the electronic properties of

a heterostructure. This model holds in the case where there is no change in potential at each surface as the interface is formed. An alternative approach is the interface dipole model, where the structure of the interface causes a shift in the entire band lineup relative to the predictions of the EAM. It is now commonly accepted that gap states induced by interface bonding would lead to such a dipole.

The main focus of our experiment was to measure the band offsets and to explore the interface dipole at the heterostructure interface. The combination of x-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS) measurements is a well-established method of determining band discontinuities at heterojunction interfaces.^{8,9} Our basic approach in this study was to obtain clean GaN surfaces through ammonia exposure at elevated temperatures and to form a Si₃N₄ layer by depositing silicon on a clean surface followed by low temperature electron cyclotron resonance (ECR) plasma nitridation. The XPS and UPS measurements are obtained after each step in the process, and yield the band bending from shifts in the gallium 3*d* and 3*p* core levels. The band offsets and electron affinities are deduced from the UPS spectra, and the contribution of the interface dipole is determined from the XPS and UPS measurements.

II. EXPERIMENTAL PROCEDURES

The GaN films used in this study were grown via metalorganic vapor phase epitaxy (MOVPE) on 50 mm diam on-axis 6*H* (0001) substrates with a conducting AlN (0001) buffer layer. The thicknesses of the GaN epilayer and the AlN buffer were 1.1 and 0.1 μm, respectively. Silicon was used as the *n* dopant, and magnesium was used as the *p* dopant. Dopant concentrations ($N_d - N_a$) of 1×10^{17} cm⁻³

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and $(N_a - N_d)$ of $2 \times 10^{18} \text{ cm}^{-3}$ were measured for the *n*-type and *p*-type samples using capacitance–voltage measurements with a mercury probe.

Ex situ surface preparation consisted of a series of three sequential dips of 1 min in trichloroethylene, acetone, and methanol, followed by immersion in 49% HCl for 10 min. The samples were then placed in the loadlock for entry into the transfer line that interconnects several analysis and processing chambers. After the initial surface analysis, the sample was moved to the gas source molecular beam epitaxy chamber (GSMBE) for *in situ* chemical vapor cleaning (CVC). The *in situ* cleaning process consisted of annealing at 860 °C for 15 min in a NH_3 atmosphere, the details of which were previously reported.^{5,10,11}

After cleaning and other process steps, the samples were transferred under UHV to the surface analysis chambers. For XPS, a dual anode source was used to generate magnesium (1253.6 eV) or aluminum (1486.6 eV) x rays. The resolution of the analyzer was determined from the full width half maximum (FWHM) of a gold $4f_{7/2}$ spectral peak to be approximately 1.0 eV; however through curve fitting, spectral peak positions could be resolved to ± 0.1 eV.

UPS with He I (21.2 eV) radiation was employed to measure the electronic states near the valence band and to determine the electron affinity. A negative 4 V bias was applied to the sample to overcome the work function of the analyzer.

To form the silicon nitride layer, silicon was deposited via MBE, and nitrided by an ECR N_2 plasma. The plasma conditions were 300 W of microwave power for 30 s, pressure of 7.5×10^{-4} Torr, and sample temperature of 300 °C.

The XPS and UPS spectra were measured to obtain information about the core levels and valence band after each of the following steps: 4 Å Si deposition, N_2 plasma of the Si layer at 300 °C, 2 Å Si deposition (6 Å total) and N_2 plasma at 300 °C, 650 °C anneal for 15 min, final 3 Å Si deposition (9 Å total) and N_2 plasma at 300 °C, and a 15 min 650 °C final anneal. XPS allows chemical bonding and band bending to be discerned by following the relative peak position shift during evolution of the experiment. Valence band information, as well as the electron affinity of each material, are determined from the UPS spectra. A combination of XPS and UPS provides information about the band discontinuities at the interface, as well as allows observation of a change in the interfacial dipole.

III. RESULTS

The evolution of the UPS spectra from the clean GaN through nitridation and final anneal of deposited 9 Å Si for the *n*-type experiment is shown in Fig. 1. The valence band maximum (VBM) of the clean GaN surface was determined from extrapolation of a line fit to the leading edge of the spectrum (Fig. 2). The VBM of the GaN and the Si_3N_4 signals were measured at 3.1 ± 0.1 and 2.3 ± 0.1 eV (referenced to the Fermi level), respectively. Because the deposited layers obscure the VBM, it is necessary to detect a more intense bulk GaN spectral feature to reference the position of the VBM. A feature at 13.4 eV in the spectra shown in Fig. 1 has

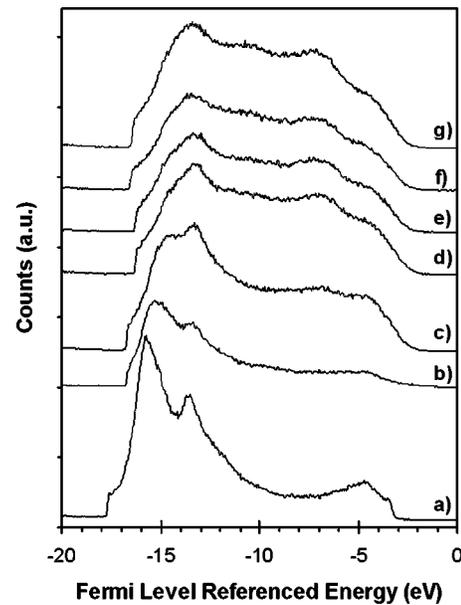


FIG. 1. UPS spectra of the valence band maximum of (a) CVC clean *n*-GaN, (b) 4 Å Si, (c) 4 Å Si and N_2 plasma, (d) 6 Å Si and N_2 plasma, (e) 6 Å Si, N_2 plasma and 650 °C anneal, (f) 9 Å Si and N_2 plasma, and (g) 9 Å Si and N_2 plasma, 650 °C anneal.

been attributed to GaN bulk excitation.¹² This feature shifts towards lower binding energy by 0.2 ± 0.1 eV with the deposition of 4 Å of Si and the nitridation that followed, and is ascribed to an increase of the band bending by 0.2 eV. Following the peak movement is only possible when the substrate emission is observable, therefore when the layer thickness obscures this emission, further information about band bending cannot be obtained. In our UPS measurements, emission from the substrate was not detected for the final 3 Å (9 Å total) silicon deposition and nitridation. With an increase in thickness, the valence band turn-on and signature peaks for Si_3N_4 remained unchanged.

The valence band turnon was measured to be 1.4 ± 0.1 eV for the *p*-type GaN material. From the doping concentration of 2×10^{18} in the *p*-type GaN, the bulk Fermi level was determined to be ~ 300 meV above the valence band maximum. This indicates significant downward band bending of 1.1 eV for the clean *p*-type GaN surface.

The electron affinity can be obtained from the UPS by determining the width of the spectra, using the relation

$$\chi = h\nu - W - E_g, \quad (1)$$

where W is the spectral width from the VBM to the low energy cutoff, $h\nu$ is the photon energy (21.2 eV), and E_g is the band gap of the material. Using 3.4 eV as the band gap, the electron affinity was determined to be 3.1 ± 0.1 eV for both the *n*- and *p*-type GaN. As we repeated these experiments, there was some variation in the low energy cutoff, which we attribute to variation in the electron affinity due to surface adsorbates. The value of 3.1 eV employed here was obtained from our cleanest surfaces, but it may yet reflect the presence of H or N adsorbates. As verification that our measured turnon is indeed the VBM, we note that our results

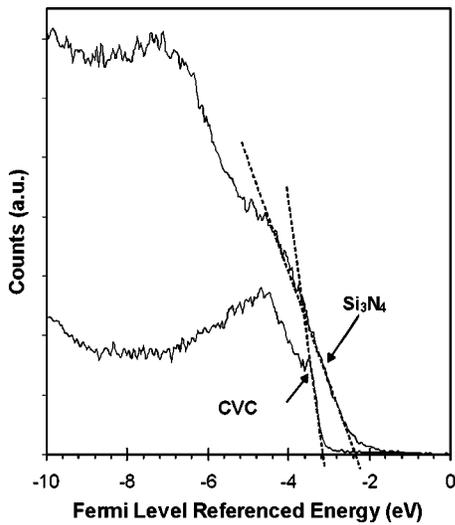


FIG. 2. UPS spectra of the valence band maximum of CVC clean *n*-type GaN and the Si₃N₄ final surface, with the valence band maximum indicated by dashed lines.

indicate that the Ga 3*d* is 17.7 eV below the VBM, which is consistent with results of Waldrop and Grant.¹³

The same approach is used to determine the electron affinity of the Si₃N₄ layer. Although the band gap of Si₃N₄ has a range of reported values,^{14,15} we will use the value of 5.3 eV and consequently obtain an electron affinity of 1.8 ± 0.1 eV. While this value is similar to that in prior reports^{16,17} of 2.1 eV, the uncertainty of the band gap of the material, as well as the ±0.1 eV measurement uncertainty, can account for the 0.3 eV deviation.

The ionization energy, *E_i*, which is the difference between the VBM and the vacuum level energies, will also prove useful in the analysis. As determined from the UPS spectra, *E_i* = *hν* - *W*. Therefore the ionization energy of the *n*-type GaN is 6.5 ± 0.1 eV, and that of the Si₃N₄ is 7.1 ± 0.1 eV.

The evolution of the gallium 3*d* peak during the *n*-type GaN experiment is shown in Fig. 3. The initial peak position for the clean surface was determined to be 20.63 ± 0.1 eV. Spectra observed after the Si deposition showed shifts that were smaller than 0.1 eV. For the final surface, which consisted of accumulated 9 Å of Si, which was nitrided, the peak was observed at 20.43 ± 0.1 eV, indicating a shift of 0.2 ± 0.1 eV for the entire experiment. This shift is consistent with movement of the bulk peak located at ~13.4 eV in the UPS spectra shown in Fig. 1.

Figure 4 presents the evolution of the gallium 3*p* and silicon 2*p* core levels during the *n*-type experiment. The Ga 3*p* core levels are consistent with the Ga 3*d* core levels in that they shift to a lower binding energy by 0.2 eV during the course of the experiment. This shift to lower binding energy is ascribed to an increase in the band bending by 0.2 eV during interface formation. The Si 2*p* peak position after the initial deposition of Si is found to be 100.03 ± 0.1 eV. After nitridation, this core level shifts towards a peak position of 102.44 ± 0.1 eV, and remains essentially constant throughout the remainder of the experiment. This large 2.44 eV shift of the Si 2*p* core level is indicative of a chemical shift due to

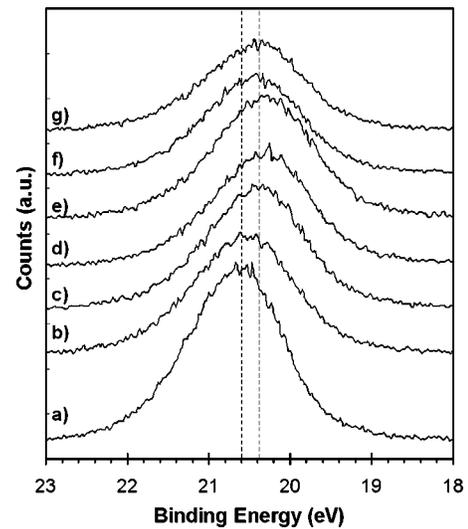


FIG. 3. XPS Ga 3*d* core level spectra of (a) CVC clean *n*-GaN, (b) 4 Å Si, (c) 4 Å Si and N₂ plasma, (d) 6 Å Si and N₂ plasma, (e) 6 Å Si, N₂ plasma and 650 °C anneal, (f) 9 Å Si and N₂ plasma, and (g) 650 °C anneal. The peak positions of the initial surface as well as the final surface are indicated by dashed lines.

Si–N bonding, and is consistent with reported values for Si₃N₄.^{18,19} In an additional approach to explore the composition of our films, we measured the energy difference between the N 1*s* and Si 2*p* core levels. For the thin films in this study the N 1*s* core level was obtained, but the Si–N peak was not resolvable due to the dominance of the nearby Ga–N peak. We prepared thicker films of Si₃N₄ on GaN using the same techniques, as well as thin films on silicon. In both cases, the energy difference between the N 1*s* and Si 2*p* core levels was found to be 295.65 ± 0.1 eV. Literature values for this difference are 295.7 eV for Si₃N₄ films, while

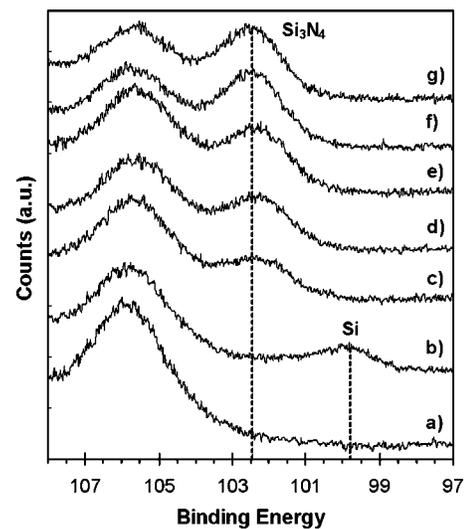


FIG. 4. XPS Ga 3*p* and Si 2*p* core level spectra of (a) CVC clean *n*-GaN, (b) 4 Å Si, (c) 4 Å Si and N₂ plasma, (d) 6 Å Si and N₂ plasma, (e) 6 Å Si and N₂ plasma, (e) 6 Å Si, N₂ plasma and 650 °C anneal, (f) 9 Å Si and N₂ plasma, and (g) 650 °C anneal. The peak position of the Si 2*p* core level after silicon deposition as well as the final surface are indicated by dashed lines.

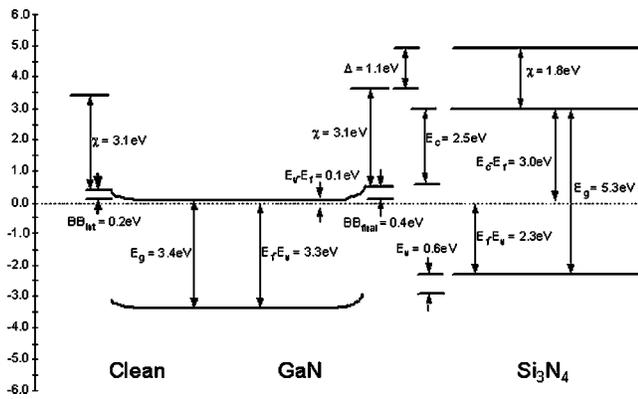


FIG. 5. Bands deduced for the clean *n*-type GaN surface (left) and the interface between *n*-type GaN and Si₃N₄. The valence band offset, E_v , conduction band offset, E_c , band bending, and interface dipole, Δ , are presented.

for SiN_{*x*} ($x < 1.33$) films a value of 295.4 eV was observed.^{19–21} Moreover, analysis of the integrated areas for the N 1*s* and Si 2*p* core level peaks yielded a N/Si ratio of 1.32 ± 0.01 . These results are consistent with the formation of stoichiometric Si₃N₄.

The evolution of the gallium 3*d* peak for the *p*-type GaN experiment was also measured. The initial peak position for the clean surface was observed at 18.88 ± 0.1 eV. After the 4 Å Si deposition and nitridation, the peak shifted to a value of 19.38 ± 0.1 eV, a difference of ~ 0.5 eV. After each process with 650 °C, the Ga 3*d* core level shifted from the value of the as deposited film by an additional ~ 0.2 eV, as evidenced by the peak positions of the Si₃N₄ formed from 6 Å total Si and plasma/650 °C anneal and the 9 Å total Si and plasma/650 °C anneal treatments shown at 19.61 ± 0.1 and 19.58 ± 0.1 eV, respectively. The purpose of the anneal is to allow reconstruction and densification of the nitride film after deposition, thereby improving the quality of the film for device fabrication.^{22,23} During the course of the experiment we observed a shift in the Ga 3*d* peak of 0.70 ± 0.1 eV. This shift is consistent with the gallium 3*p* core level, suggesting that the change in core level is due to a change in band bending.

IV. DISCUSSION

The method used for determining the valence band offset is similar to that of Waldrop and Grant and of Kraut *et al.*²⁴ Their basic approach was to reference the VBM to a core level in the XPS spectra of each semiconductor and to use the measured difference between the core level energies to discern the band discontinuities. In our study, we use UPS to measure the energy of the VBM relative to the Fermi level, and XPS is used to obtain band bending information by measuring the shift in core level energy relative to the Fermi level. A combination of these two photoemission techniques provides band alignment at the heterojunction interface.

Figure 5 shows the proposed band lineups for the *n*-type GaN/Si₃N₄ interface. Valence band offset (VBO) determination is the measured UPS turnon for GaN (3.1 eV), minus the Si₃N₄ turnon (2.3 eV), minus the band bending (0.2 eV).

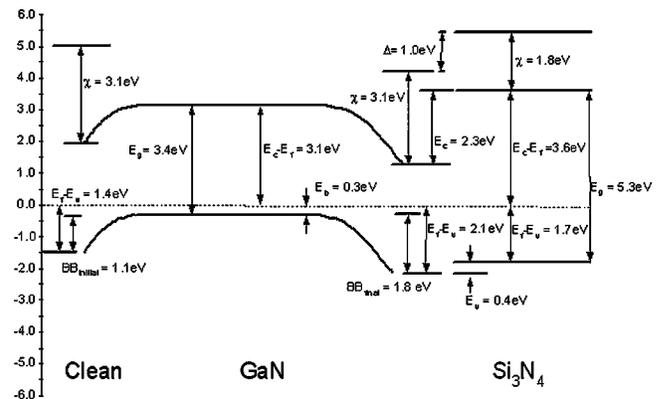


FIG. 6. Bands deduced for the clean *p*-type GaN surface (left) and the interface between *p*-type GaN and SiO₂. The valence band offset, E_v , conduction band offset, E_c , band bending, and interface dipole, Δ , are presented.

This value, along with knowledge of the band gap of the material, allows the CBO to be deduced. The VBO is found to be type II band alignment, where the valence band of the Si₃N₄ is 0.6 ± 0.1 eV above the GaN VBM, and the CBO is 2.5 eV. Figure 6 shows the proposed band lineups for the *p*-type GaN/Si₃N₄ interface. The UPS turnon for the clean GaN and the Si₃N₄ was observed at 1.4 and 2.2 eV, respectively. XPS spectra showed a change in downward band bending of ~ 0.7 eV during formation of the interface. The VBO is again found to be type II band alignment 0.4 ± 0.1 eV above the GaN VBM, and the CBO is 2.3 eV.

The measured electron affinities for GaN and Si₃N₄ are represented in Figs. 5 and 6. The electron affinity model of heterojunction formation assumes that the vacuum levels would align at the interface. Our results show a deviation from the EAM of 1.1 and 1.0 eV for the *n*-type GaN and *p*-type GaN substrates, respectively. Note that this deviation is determined directly from the difference in measured ionization energy minus the measured band offset. The EAM model is based on the premise that the interface is formed without disruption of the surface electronic states of either of the two materials. The measured difference between the prediction of the EAM and the experimentally observed band offset represents a change in the interface dipole.

As an alternative to the electron affinity model, it may be considered that the heterojunction band offsets are determined by alignment of the charge neutrality levels (CNLs) of the two materials. The charge neutrality levels represent the branch point of the surface (or interface) states since they are related to the valence or conduction band. Charge can transfer between the interface states of the two materials, which will cause an interface dipole. The band offset will be determined by the relative position of the CNL of the two materials if the density of states is high or if the CNL of the two semiconductors is similar in relative energy.

Robertson¹⁶ adapted the Schottky barrier interface defect model presented by Cowley and Sze²⁵ to employ CNLs as the pinning levels at a heterojunction interface. This model was used to analyze silicon/oxide interfaces, and the model seems consistent with most experimental results. This model is given by

$$\varphi_{\text{CBO}} = (\varphi_{\text{CNL},a} - \varphi_{\text{CNL},b}) - (E_{g,a} - E_{g,b}) + S\{(\chi_a - \chi_b) + (E_{g,a} - E_{g,b}) - (\varphi_{\text{CNL},a} - \varphi_{\text{CNL},b})\}, \quad (2)$$

where φ_{CBO} is the CBO, χ and φ_{CNL} are the electron affinities and charge neutrality levels of each semiconductor (*a* and *b*), respectively, and *S* is a pinning factor based on the dielectric properties of the materials. Here, φ_{CNL} is defined relative to the VBM of each semiconductor. A value of *S* = 1 represents the EAM while a value of 0 represents pinning at the CNL levels. To our knowledge, the CNL of Si_3N_4 has not been reported. Using the value of *S* for the Si_3N_4 -Si interface (0.51) and the measured band offset from previous work,^{16,23} we can deduce the CNL of Si_3N_4 to be 1.5 eV above the valence band maximum. While more research is necessary to assign a CNL value for Si_3N_4 , it is reasonable to consider this prediction of the valence band offset for comparison to our experimental results. Monch²⁶ has reported the CNL of GaN to be 2.37 eV above the valence band maximum. Although the dielectric screening parameter *S* has not been determined for the GaN/ Si_3N_4 interface, within the limits of *S*=0 and 1 the valence band types and offsets would be type II 0.9 eV and type I 0.9 eV, respectively. If the assumption is made that the parameter *S* is similar to that for the Si/ Si_3N_4 interface (0.51), the CNL relation given in Eq. (2) predicts the valence band offset to be ~0.1 eV (essentially no offset) for the GaN/ Si_3N_4 interface. Conversely, the dielectric screening parameter can be deduced for the interface using our results and the CNL of GaN and Si_3N_4 . A value of *S*=0.26 is obtained for the GaN/ Si_3N_4 interface.

This prediction, as well as our results, are significantly different from the results of Nakasaki *et al.*,³ who reported type I band alignment with an offset of 1.0–1.2 eV for the GaN/ Si_3N_4 interface. A factor that could play a major role in this difference is the cleaning method used for GaN. Their studies used a NH_4OH etch and a combination of H_2 and N_2 plasmas for *in situ* surface preparation. While the oxygen content was greatly reduced from that in the as-loaded case, a significant amount remained after surface preparation, suggesting Ga–O bonding.³ In a previous study,¹⁰ the GaN/ SiO_2 interface was examined via photoemission, and showed type I alignment and a VBO of ~2 eV. We suggest that Ga–O bonding exists at the GaN/ SiO_2 interface and contributes to the large offset and interfacial dipole change. Our study begins with a clean GaN surface (contamination levels of <1% for oxygen and carbon) that allows the GaN/ Si_3N_4 interface to be measured more precisely.

In an attempt to understand the relationship between of our measured band alignment and the different models for heterostructure band alignment, in Fig. 7 we compare our measured interface alignments to experimental results for Si_3N_4 on Si.^{16,22,23} In both cases the diagrams are aligned to the vacuum level at Si_3N_4 , which has been measured to be at the same energy relative to the silicon nitride bands. The band gap of each material is indicated, as is the VBO. The position of the vacuum level of the clean semiconductor surface is indicated, and the difference between these values and the surface vacuum level is the deviation from the EAM.

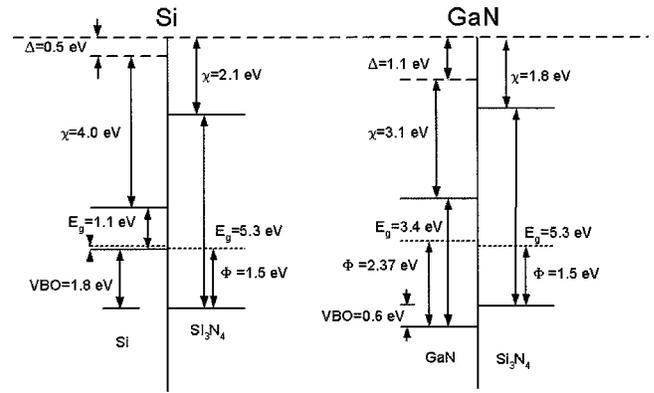


FIG. 7. Band alignment of Si/ Si_3N_4 and GaN/ Si_3N_4 interfaces. The dashed line at the top corresponds to the electron affinity of the Si_3N_4 surface, which is common in both interfaces. The deviation from the electron affinity model is shown by Δ , and the charge neutrality level is indicated by a dashed line within the band gap. The VBOs are determined from the measurements and Δ is the averaged values.

This difference represents the change in interface dipole, and was found to be 0.5 and 1.2 eV for Si_3N_4 on Si and GaN, respectively.

Also indicated in Fig. 7 is the CNL of the semiconductors.^{16,26} Additionally, the predicted CNL of Si_3N_4 (1.5 eV) deduced as described above is also presented. We observe that the CNLs nearly align for the GaN/ Si_3N_4 interface, suggesting correlation of this interface with the CNL model with low dielectric screening parameter *S*. The progression of the interface dipole deduced from the deviation from the EAM is most likely related to changes at the semiconductor surface since the silicon nitride is the same in both cases. For the Si/ Si_3N_4 interface, the Si surface reconstruction is expected to change during the formation of the nitride layer. This effect alone could account for the small change in interface dipole, and the same could be true for the GaN/ Si_3N_4 interface. For GaN/ Si_3N_4 , we expect Ga–N–Si bonding exists within the initial few monolayers at the heterojunction interface. Because of the similarity in bonding at the interface we may expect a smaller interface dipole than that of the GaN/ SiO_2 interface. This indeed is the case where we find an 1.1 ± 0.1 eV interface dipole for GaN/ Si_3N_4 and a 1.7 ± 0.1 eV one for the GaN/ SiO_2 interface.

V. CONCLUSIONS

The surface and interface properties of *n*- and *p*-type GaN/ Si_3N_4 were systematically investigated by photoemission techniques and band alignment information was obtained. Annealing in ammonia at 860 °C provided clean stoichiometric GaN surfaces with ~0.2 eV upward band bending and ~1.1 eV downward band bending for the *n*-type and *p*-type surfaces, both with an electron affinity of 3.1 eV. For GaN/ Si_3N_4 , type II band alignment was observed and valence band offsets were measured to be $\sim 0.5 \pm 0.1$ eV for both *n* type and *p* type. The interface dipole deduced by comparison with the electron affinity model was 1.1 ± 0.1 eV. The charge neutrality model provided a reasonable description of the band alignment of the GaN/ Si_3N_4 interface. It is suggested that the presence of oxygen at

the interface could substantially change the band offsets. These results indicate that Si_3N_4 should passivate *n*-type surfaces, but may not be appropriate for passivation of *p*-type surfaces.

ACKNOWLEDGMENTS

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