Abstract

A novel Photoluminescence (PL) model for the effect of 1 MeV electron irradiation on AlGaN/GaN with a variation in Si_3N_4 passivation layer thickness has been developed by examining the transitions and changes in defect populations and energy levels.

The PL results of Si_xN/AlGaN/GaN gives information on the spatial localization of impurities such as oxygen and silicon, which are precursors to the D^0 X centers, deeper impurities like magnesium, and V_n and V_{Ga} donor information.

The Si_3N_4 passivation layer shows a mono-atomic variation with PL intensity prior to 1MeV radiation. The post radiation Pl gives a 50nm peak and a 20 nm minimum in the deep center range, but then reverses to mono-atomic variation in the near band edge range. There is a shift in the main D^0 X center in the rear band edge due to mismatch lattice constants which results from tensile strain.

The model that follows seeks to explain the observed changes in the PL due to 1 MeV electron irradiation. The changes with Si_3N_4 thickness pre-irradiation are explained as due to the attenuation of the PL laser beam going through the material, and corresponded linearly to the thickness of the Si_3N_4 pre-irradiation, but not post irradiation.

Introduction

AlGaN/GaN heterostructures have great promise in a variety of high power and fast switching applications. Much of this is owing to the high electron mobility of the 2DEG (1880 $cm^2V^{-1}s^{-1}$). Comparable GaN transistors have been shown to have an "on" resistance lower than silicon by orders of magnitude. Devices used in space borne applications experience both protons and electrons from the earth's radiation belt. The space environment in which these AlGaN\GaN High Electron Mobility Transistors (HEMT's) need to operate requires that they be operational under the equivalent of 1 MeV electron irradiation. [ICRU Report No. 37, 1984] High energy particles cause displacement damage, which can become electron or hole traps; more rarely, donors or acceptors. For 1 MeV electron irradiation (EI) the dominant defect produced is a 0.06 eV donor, which is a nitrogen vacancy, and which was identified using Hall Effect measurements (Look et al, 1997]. Previous studies have been done with electron irradiation on RF GaN HEMT's that characterize their degradation [Kalavagunta, 2009]. Other studies have discussed the role of bulk traps in device degradation [Meyer, 2008; Fang et al, 2011; Polyakov et al, 2008]. None of these studies exclusively included the role of the Si_3N_4 thickness in the formation of the surface states, either intrinsically or following irradiation.

The present study was undertaken to determine the effect of the variation of Si_3N_4 buffer layers combined with electron radiation on AlGaN/GaN heterostructure High Electron Mobility Transistors (HEMTs). Theory suggests that the V_N defect has a level in the conduction band (CB) which when occupied, auto ionizes into a hydrogenic configuration with an energy about 30-40 meV below the conduction band. The donor and acceptor created in 1 MeV irradiation are strongly believed to be donor and acceptor components of the N Frenkel pair, that is, the N vacancy and the N interstitial. The model given by Look confirms the expected donor nature of V_N and demonstrates the rare appearance of an (N_I) as an acceptor. [Polenta et al, 2000]

V_{GA} is often the dominant acceptor in undoped GaN. After 1 MeV irradiation, both the number of acceptors and donors increase by an amount that is ~ 1 cm^{-3} by each bombarding electron per cm^2, which gives a production rate of ~1 cm^{-1} . The vacancy is thought to be V_N, a N vacancy, and the acceptor an N interstitial, N_I. The donor activation energy E_D is .06 eV, making V_N a shallow donor. [Look, 2001]

Experiment

The effect of passivation layer thickness was investigated using various thicknesses (0, 20, 50 and 120 nm) on bare epilayer AlGaN\GaN structures Photoluminescence (PL) was accomplished using a HeCd laser (325 nm) as excitation source with an emission detection range varying from 3550 to 7450 Å. The PL spectra were measured using a Spex 1250M spectrometer with a 2400 grove/mm grating blazed at 3000 Å, typical for wide-band-gap applications. Samples from each wafer were pre-characterized in order to establish a baseline and to observe the variation in radiative native defect centers owing to fabrication method. Post-radiation PL were taken using a 266-nm laser. This data has been normalized relative to the near band edge peaks. The 266 -nm laser was normalized with respect to the 325 laser when their data was compared. Penetration depths were assumed to vary as $1/e^{\alpha d}$ where $\alpha = 2.25 \times 10^6$ cm^{-1} for Si_3N_4 and is about 10^5 cm^{-1} for GaN. Photoluminescence can give information of the impurity as well as other donor and acceptor energies. The post-irradiation PL peaks give a good indication of how the irradiation has changed the donor-acceptor population and can help to explain post-radiation Hall measurement results, as well as the radiation induced defects that lead to decreased conductivity and increased leakage current.

Discussion

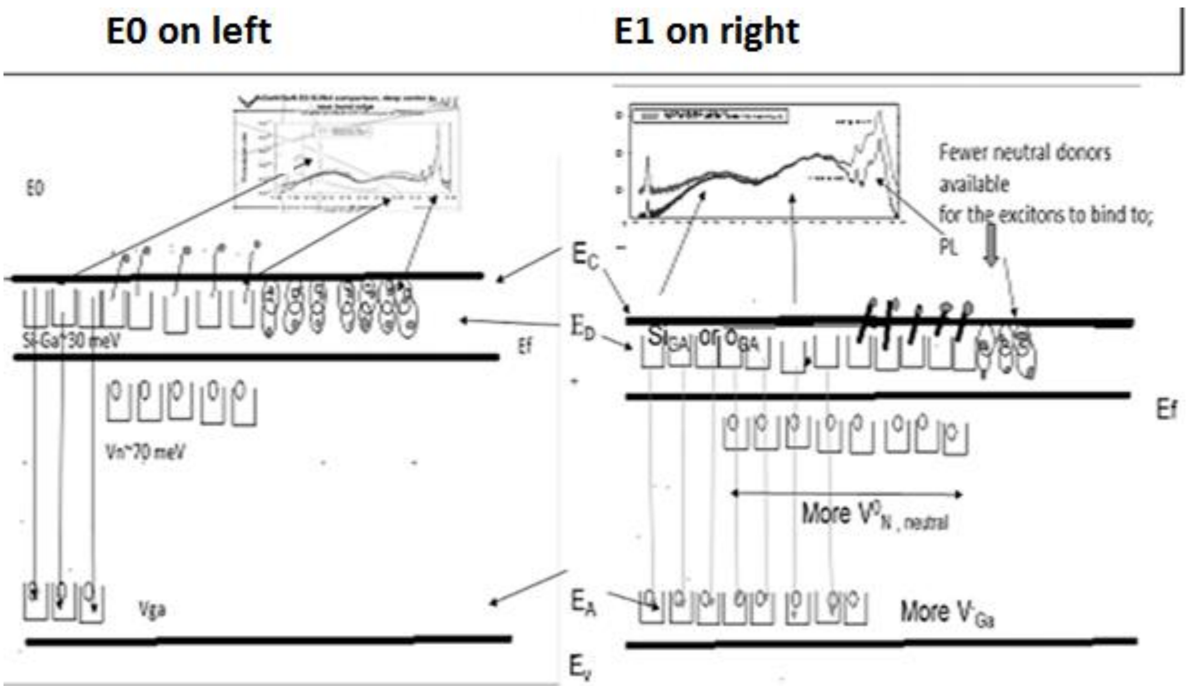

Figure 1 Model for radiation damage explaining PL peak changes and change in the Nitrogen and Gallium donor and acceptor populations.

The model in Figure 1 summarizes the PL radiative peak production events before and after 1.0 MeV electron. The diagram on the left is for pre-irradiation (E0), and on the right is for post irradiation (E1). For E0, below the conduction band, there is the donor level, $E_{D,}$ which starts at approximately 30 meV; the donors here would be shallow donors. Above the valence band is the acceptor level E_A. Silicon is a known impurity in AlGaN/GaN, as well as oxygen. They are small shoulders off of the peak at 3.47eV. At approximately 30meV, a positively charged, a silicon on gallium, $Si^{+}{}_{Ga}$, will drop to the acceptor level, E_A, at a rate in accordance to its temperature dependence. There are also Si^{+}_{Ga}, just below the conduction band in energy in the E_D level and gallium vacancies, V_{GA} just above the conduction band in energy in the E_A level. The nitrogen vacancies, V_N, which are closer to mid-state, will retain their electrons because they are below the Fermi level, at approximately 70 meV.

Excitons, shown as the upper circle of the pairs on the right on the E_D level, bind to neutral donors, which are shown as the circles attached to them. Here the Si atom is neutral on Ga, Si^0_{Ga} excitons seek out and bind to neutral donors. Bound exciton recombination dominates over free electron recombination in less pure material [Jackson, H, 2014]. Here it is proposed one is observing Si^0_{Ga} because the donors with the paired excitons are neutral as revealed in the near band edge PL peak, Figures 1 and 2.

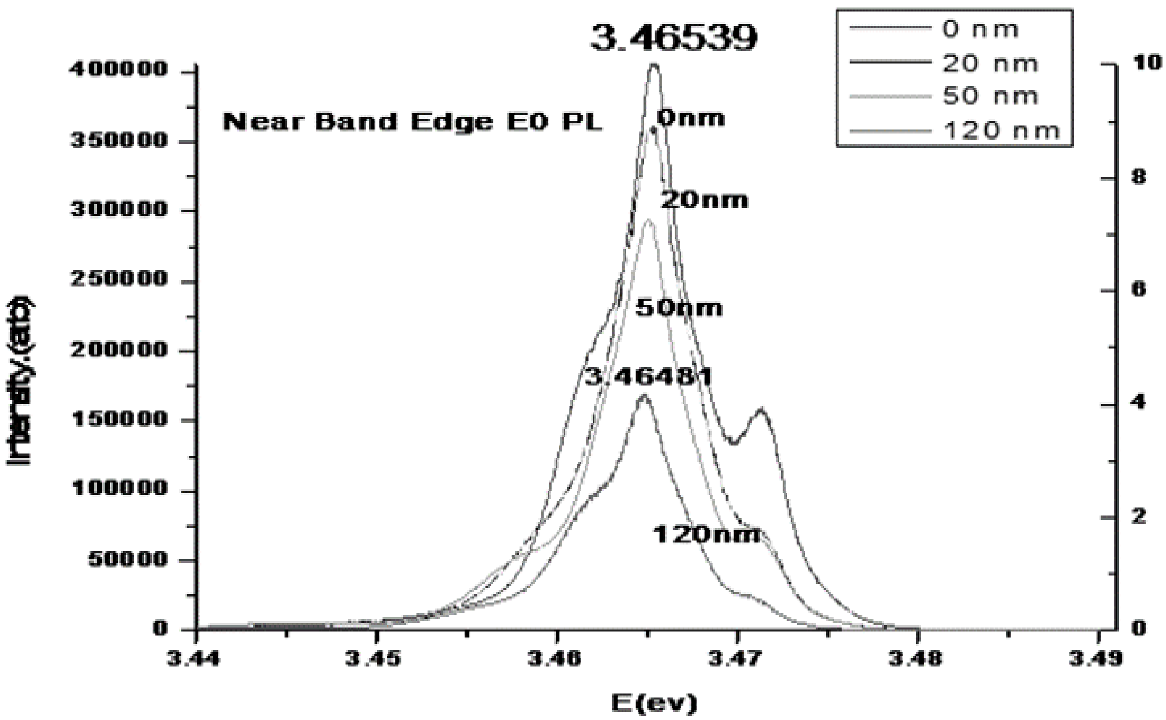

Figure 2. The near band edge of the samples showing a mono-atomic attenuation of the PL light with Si_3N_4 thickness.

There are many neutral donors with which excitons can bind to in this area, so the PL peak is high in the near band edge area (in the insert plot for E0 in Figure 1). While this model is showing Si as the neutral donor, but both silicon and oxygen peaks show up in the NBE peaks; oxygen (3.46 eV) and silicon (3.466 eV). Other models may propose oxygen as the neutral donor. The Pl signal in general is proportional to an E_D-E_A model that will be shown in equations 1 and 2.

The Yellow line. Unintentional doping in AlGaN/GaN is due to shallow donors, and PL results on the samples in this study imply that these donors are oxygen or silicon [Neugebauer and Van de Walle, 1996; Mattila and Nieminen, 1997; Lee et al, 1997; Kwon et al, 2000]. There are many models invoking defect complexes and substitutional sites, but Colton [Colton, 2000] believes unintentional silicon is replacing nitrogen (Si_N) or oxygen replaces nitrogen (O_N). Based on the effective mass of GaN, the hydrogenic donor binding energy was calculated to be E_D = 33 meV, comparable to the ionization energies of for Si_{Ga} = 30.8 meV and O_N = 32.4 meV. The exciton Bohr radius α was calculated to be 0.529 Å $(m_0/m^*)\varepsilon$ = 23 Å . There is a large amount of evidence (Colton, 2000) that supports a donor-acceptor pair (DAP) transition. The resulting emitted photon from the recombination is defined by:

$$\hbar\omega = E_g - E_A - E_D + e^2 / (\varepsilon R) \qquad (1)$$

Here E_g is the band gap energy of ~3.47, and E_A and E_D are the acceptor and donor binding energies, respectively. In the last term, R is the distance between the donor and acceptor which defines the Coulombic attraction between the donor and acceptor charge states. To be noted the V_{GA}, an acceptor defect, involved in emission in the yellow spectral region (thus Yellow Line, or YL transition), has the lowest formation energy of any native defects in n-GaN. A donor acceptor pair transition occurring during PL defined by equation 1.

The Blue Line**.** Emission in the blue region of the visible spectrum is believed to be due to a transition involving a complex with Mg. The presence of Mg in n-GaN is a result of its processing. The Mg acceptor on a gallium site (Mg_{GA}) is believed to have a hydrogenic binding energy of about 200 meV, with some reports indicating a value up to 250 meV [Kwon et al, 2000). Using equation 1, as done for the donor site above, but instead for a hole and using the effective hole mass, the acceptor Bohr radius is estimated to be 4 Å. As it is for the YL, there are a number of models that define the BL transition occurring. The one that best fits the PL spectra in this research is the $Mg_{GA} - V_N$ transition [Reshchikov and Markoc, 2005].

Radiation Effects. For the post irradiation, E1, shown on the right side of Figure 1, the near band edge centers are much lower and have degraded as is shown in Figures 3 through 6.

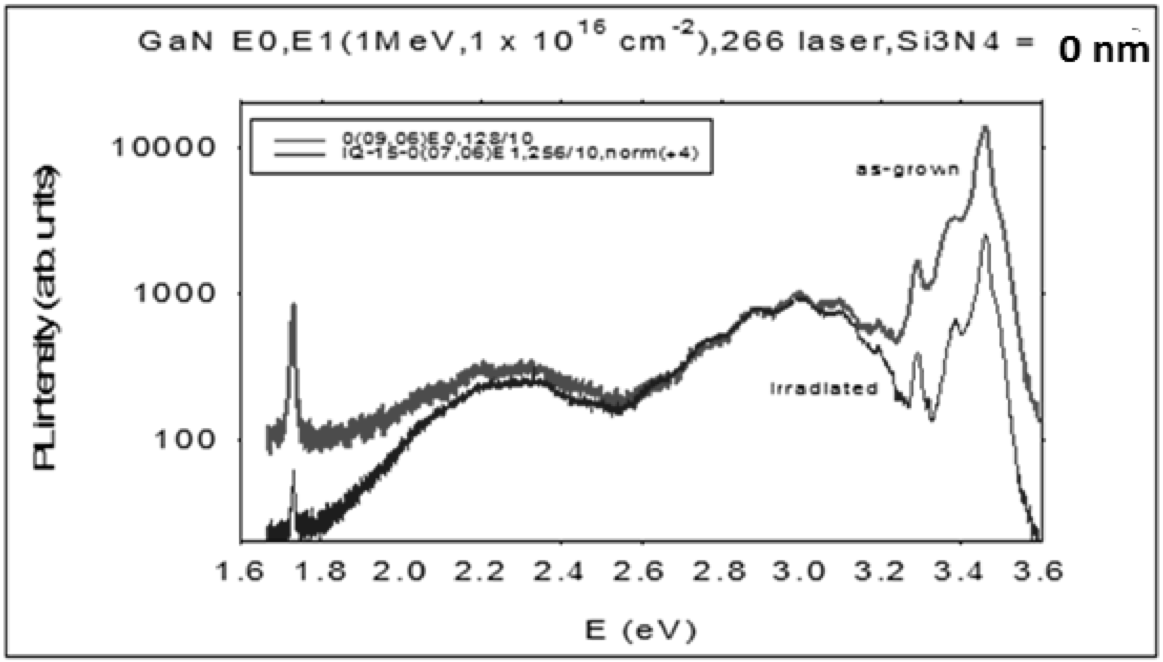

Figure 3. PL from unpassivated samples after 1-Mev irradiation. Deep centers are not affected as much as shallow centers by irradiation.

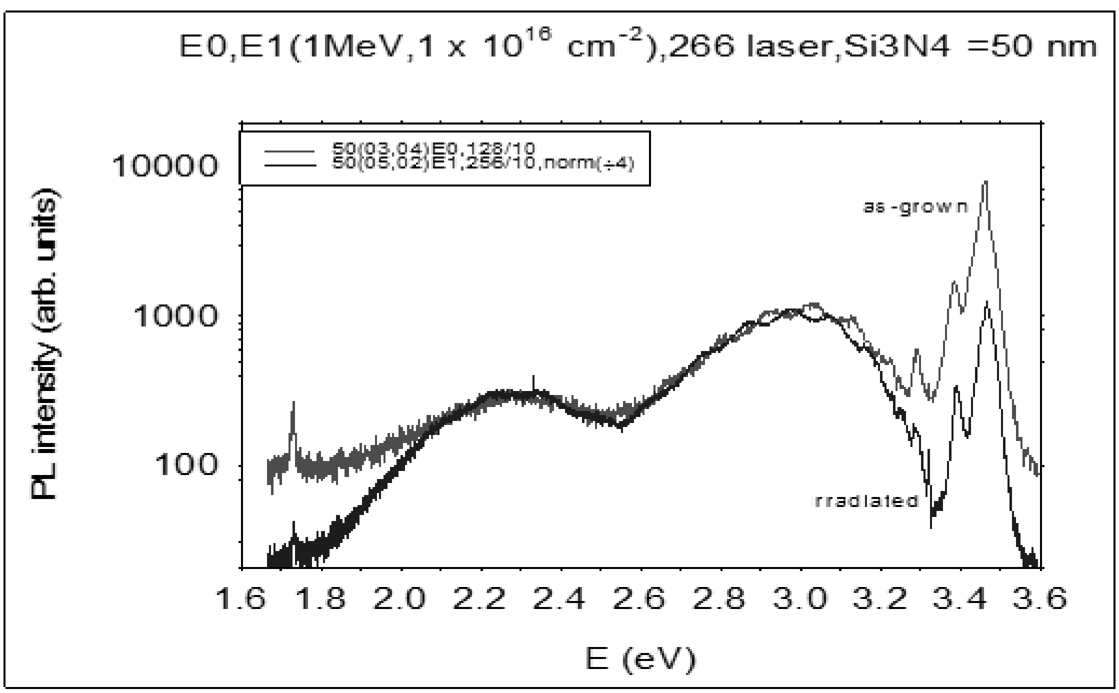

Figure 4. PL from sample with 50 nm passivation layer after 1-MeV irradiation. Deep centers are not affected as much as shallow centers by irradiation.

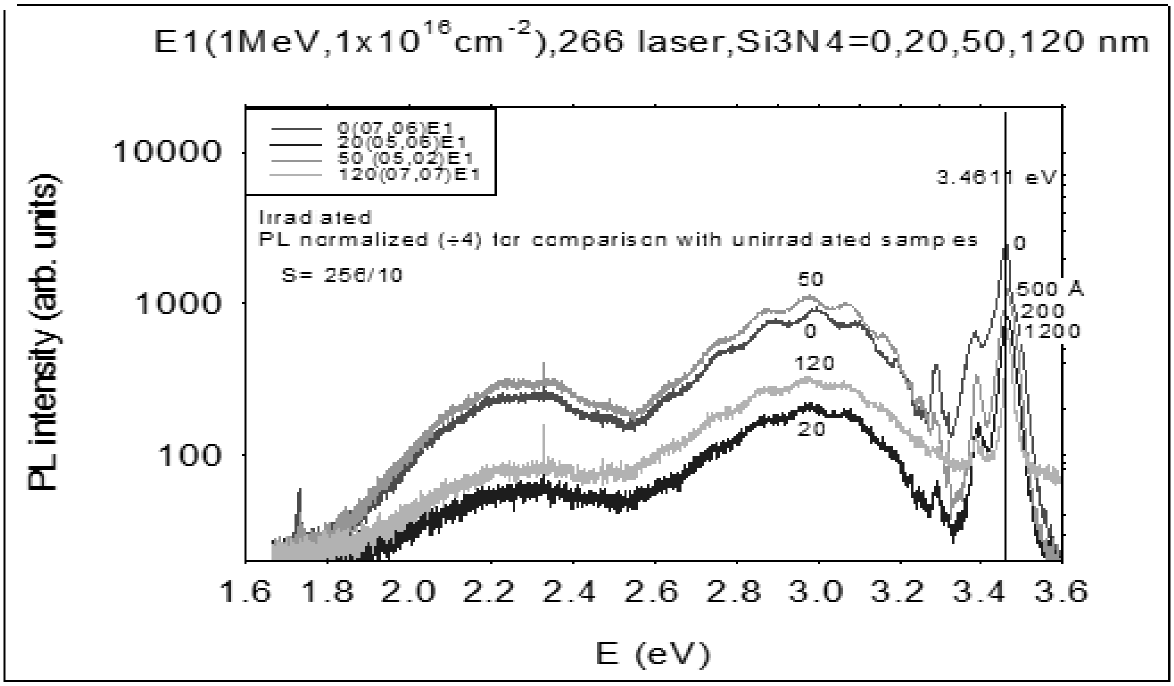

Figure 5. PL taken after 1 MeV irradiation showing deep center to near band edge region. When comparing the near band edge area with Figure 2, which is further blow up in Figure 6, the peak heights have shifted for the 20 and 50 nm passivated samples.

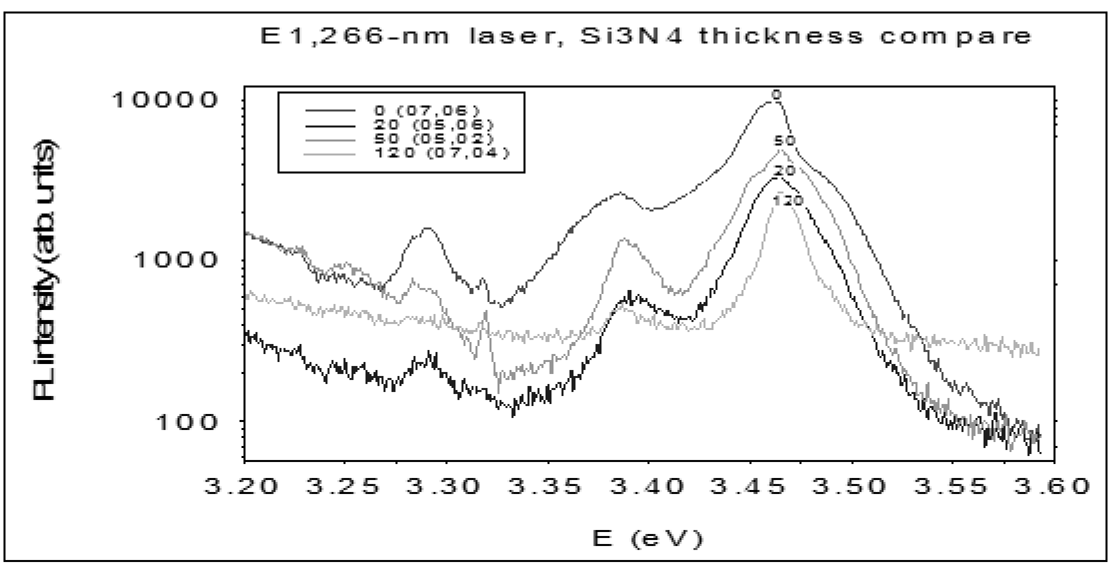

Figure 6. PL taken after 1 MeV irradiation for the emission region from 3.20 to 3.60 eV, which includes the near band edge.

Figures 3 and 4 compare the normalized pre and post irradiation PL for an unpassivated and the 50 nm passivated sample respectively. It could be expected that the shallow centers sustain more radiation induced changes, since with depth there is attenuation, according to $e^{-\alpha d}$.

Before the irradiation, the peak intensities of both the YL (2.2 eV) and BL (3.0 eV) changed monotonically with Si_3N_4 thickness. The irradiation has changed the shallow donor and defect concentrations that produce the YL and BL transitions. This tells us what the radiation produced defects are. The change in Hall carrier densities, the defect production algorithms, and the DLTS in parallel studies [Jackson, 2014] did concur with the radiation induced changes. The post 1-MeV electron irradiated PL that includes the NBE region is shown in Figure 6. Notice that in addition to being degraded, the near band edge peaks are broadened by the irradiation, indicating possibly lattice displacement damage. The NBE degradation relative to the un-irradiated for the NBE PL is evident in Figures 3 and 4 for no passivation and 50-nm passivation. In Figure 6, there is a greater degree of peak degradation in the near band edge.

With shallow center peaks, due to the collapse of exciton bound to neutral donor, less of these pairs are available. The model indicates fewer neutral Si, and fewer centers that the excitons can attach themselves to. So the PL signal is lower. Post irradiation, there is still a large amount of silicon and/or oxygen atoms, although their electrons may have excited to a higher state; some will remain neutral. Looking deeper in energy, when the sample is irradiated- the result is the creation of many V_{Ga} and V_N vacancies. For the V_{GA} in E_A, they now all may have electrons. The electrons from the Si^0_{Ga} and Si^+_{Ga} all transition to additional acceptors created in the E_A level. With the V_N electrons, they drop down to form V_{Ga}-, negatively charged. Now $V_N \rightarrow V_N^+$, as electrons have been emitted.

So the model is assuming that the deep centers are Ga (YL) or nitrogen (BL) vacancy related. In the case for the YL, the electron radiation is creating more V_{Ga}, but not enough to affect the intensity of the PL illumination, as can be seen in the post irradiation E1 plot inset on the right side of Figure 1, which is also Figure 3. This indicates either saturation occurring at 2.2 eV or there are now less of the other atoms in the complex that form the transition. The near band edge peak results from an exciton bound to a D^0X collapse. The models show V_{Ga} taking electrons from the Si, but it could also be a $V_{Ga} \rightarrow O$ transition.

Post irradiation, the amount of silicon in the GaN may not be changing, but there are V_{Ga} because 1 MeV electrons create $V_{Ga.}$, as well as V_N. While actually more nitrogen vacancies are created-they are electrically neutral so the creation of the V_{Ga} will have more of an effect.

This models analysis of the BL area is that the transition $V_{N\text{->}}$ Mg_{Ga}, which creates the PL peak at ~3.0 eV, may not lead to a decrease in peak height because the radiation may not be affecting the Mg. Mg is needed in the transition, and the radiation is not creating more Mg, but it is creating more V_N. So the BL in the plot insert on the right of Figure 1 for E1 is not changed.

If $V_{Ga\text{ ->}}O_N$, or $V_{Ga\text{ ->}}Si_N$ is producing the YL, there is enough O or Si for PL peak formation post irradiation in the 2.2 eV area, and peak doesn't change as significantly. The Pl peak intensity won't change as much if the donor population is not strongly affected by the radiation; the subsequent complexing centers necessary for the transition to occur at that energy are not strongly reduced.

The model in Figure 1 for the effects of 1.0 MeV electron irradiation on the PL can be summarized by an energy conservation equation. Equation 2 is an expansion of Equation 1 as it relates to this model, and it also gives insight into the DAP changes occurring post radiation that effect other device characteristics:

$$\mathbf{E_{Donors,\,E1} + E_{Acceptors\,E1} + E_{Dxo,\,E0} = E_{Donors,\,E0} + E_{Acceptors,\,E0} + E_{Vn,\,E1} + E_{NI,\,E1} + E_{VGa,\,E1} + E_{GaI,\,E1} \pm \hbar\omega + E_{formation} + E_{Dxo,\,E0\text{-}E1}} \quad \mathbf{(2)}$$

$E_{Donors,\,E1}$ is the post irradiation energy of the donors, $E_{Acceptors\,E1}$, is the post irradiation energy of the acceptors, and $E_{Dxo,\,E0}$ is the pre-irradiation energy of the D_{x0} centers. $E_{Donors,\,E0}$ is the pre-irradiation energy of the donors, $E_{Acceptors,\,E0}$ is the pre-irradiation energy of the acceptors, $E_{Vn,\,E1}$ is the post irradiation energy of the nitrogen vacancy, $E_{NI,\,E1}$ is the post irradiation energy of the nitrogen interstitial, $E_{VGa,\,E1}$ is the post irradiation energy of the gallium vacancy, $E_{GaI,\,E1}$ is the post irradiation energy of the gallium interstitial, $\hbar\omega$ is from equation 1, and $E_{Dxo,\,E0\text{-}E1}$ the D_{x0} change in energy.

The phonon energy $E_{\hbar\omega}$ in equation 2 is energetically costlier when it is positive (+) which would mean it is a phonon absorption. If the term is negative (-), there is a phonon emission. The samples studied where n-GaN, so the assumption can be fairly made that they are donor dominant. Table 1 summarizes the traps observed for as grown AlGaN/GAN, and their distance from the conduction band as identified by other sources.

General description	Distance from CB	source
Deep level	1.8 eV and 2.85 eV	Klein et al.
Lattice dislocation	0.5-0.6 eV	Polyakov
Nitrogen interstitials/Gallium vacancies	1.0 eV	Polyakov
Nitrogen vacancy	0.18-0.27 eV	H.K. Cho et.al, Z.Fang ,Polenta, D. Look
Nitrogen antisite	0.5 -0.6 eV	H.K. Cho et.al , D. Polenta
YL/acceptor defect/Ga vacancy	2.2 eV	Massashi Kubota, Resshikov, E.Calleja .et al.
BL	2.8 eV	Massachi Kubota
(Via DLTS)	0.58 and 1.1 eV	T. Ogino
AlGaN/Nitrogen vacancy	0.85 eV	Fang et al.
AlGaN (irradiation induced)	0.33, 0.38 eV	Hogsed et al.

Table 1 Trap Location summary

Radiation effects summary. For the Pl data in this study, with each post irradiation observed change in PL peak, the results are summarized below in Table 2. The **E1** column shows the radiation induced changes that have affected donor/acceptor population.

	E0 0 to 120 nm Si_3N_4	**E1** 0 to 120 nm Si_3N_4
Si (shallow donor)	3.466 eV /(30meV below CB)	Exciton collapse –pairs ↓PL↓
Si^+_{Ga} or O_{Ga}	NBE-E_D /(30meV below CB)	PL↓ donor electrons to E_A
Si^0_{Ga}	E_D /(30meV below CB)	Electrons excited to CB amount↓ PL ↓
O (shallow donor)	NBE-3.46 eV/(30meV below CB)	Electrons excited to CB amount↓ PL ↓
BL	3.0 eV	E1 increasing V_N
V^+_N	70 meV –below E_f	E1 increasing
YL	2.2 eV (shallow acceptor)	*E1 increasing V_{Ga} So Pl not changing
Phonon peaks	~93 meV from DX	Shifted, degraded due to E1 displacement damage
Free exciton	3.478 eV	collapsed
V_{Ga}	E_A	Increased due to E1

Table 2. Pl Peaks for AlGaN/AlN/GaN, summary of the defect peaks. * If donor population is not strongly affected by E1, PL won't change much.

Conclusion

A novel photoluminescence model has been developed which shows the changes in the donor acceptor population in Si_xN/AlGaN/GaN. By comparing the data shown for the un-irradiated versus irradiated samples (Figures 3 and 4), it is clear that the intensities of the peaks have changed. Before the irradiation, the peak intensities of both the YL (2.2 eV) and BL (3.0 eV) changed monotonically with Si_3N_4 thickness in Figure 2. The irradiation has changed the shallow donor and defect concentrations that produce the YL and BL transitions. Electron irradiation creates dislocation damage in the crystal lattice, which shifts the donor-acceptor population statistics. The PL spectrum can then give location information and thus what the radiation produced defects are. The post radiation broadening of the peaks in the NBE region verifies possible displacement damage to the lattice. The figures that compare the pre irradiation with post irradiation (Figures 3 and 4) clearly show peak degradation due to irradiation. The depth dependence or attenuation effects are illustrated in Figure 6, where there is a greater degree of peak degradation in the near band edge. Several studies in this same research have determined that the 20 nm passivation layer samples are highly anomalous due to processing irregularities, so this thickness of passivation layer gives unreliable information.

Clearly in Figure 6, the electron irradiation is destroying the components of PL peak formation at the DX center peak, perhaps by ionizing the neutral donors that the excitons attach to. Additionally, in the deep center, the YL peak is degraded post-irradiation. The E_A for the 2.2 eV YL is attributed to V_{GA}, but the peak intensity for the 3.0 eV BL increases. It has been shown in the literature as well as with this research that V_N is the dominant radiation induced defect produced throughout the structure. Radiation increases the V_{GA} production also, but perhaps the ratio of either O or Si that can cause the peak has been altered due to the radiation. The peaks are related to the energy of the donors or acceptors in the transitions. V_N is below the Fermi level and is neutral.

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