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Effect of HfO_2 Passivation Layer on Light Extraction Efficiency of AlInN Nanowire Ultraviolet Light-Emitting Diodes

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One of the probable reasons behind the limitation of light extraction efficiency (LEE) in III-nitride nanowire (NW) deep ultraviolet (UV) light-emitting diodes (LEDs) is the presence of the high surface density states that significantly contribute to the non-radiative recombination near the surface. Herein, we investigate the LEE of a single AlInN NW UV LED in the entire UV wavelength regime using finite-difference time-domain simulations. It is found that these LEDs favor transverse-magnetic (TM) polarized LEE over transverse-electric (TE) polarized emission. Further, we examine the role of the HfO_2 surface passivation layer in the improvement of LEE of AlInN NW LED at ~282 nm wavelength. Our results show that the TM-polarized LEE of such LED without any passivation is only ~25.2%, whereas the maximum recorded LEE is ~40.6% with the utilization of 40 nm HfO_2 passivation layer. This study provides a promising approach for enhancing the LEE of NW UV LEDs.

Introduction

With the increasing demand for low-cost deep ultraviolet (UV) light systems due to their diverse applications, there has been an increasing proportional need for improved UV LED performance (1, 2). III-Nitride semiconductor alloys, especially AlGaN and InGaN, have drawn significant attention due to their direct and wide bandgap energy, light emission capability for the entire UV region (3). Several efforts have been made on AlGaN planar and nanowire (NW) LEDs to improve their performance, but the performance is still limited in the deep UV region. The probable reasons for the poor performance may be the poor quality of epitaxial growth includes high threading dislocation density, electron leakage, low light extraction efficiency (LEE), and others (4, 5). Though AlInN can be optically tuned to emit the light from the deep UV to mid-infrared (IR) region, it is relatively unexplored compared to other III-nitride alloys. Recently, we have successfully demonstrated the first AlInN core-shell NW UV LEDs with a relatively high IQE of ~52% (6-9). However, the LEE study of such NW LEDs is unexplored to the best of our knowledge. In this context, we have studied the LEE properties of a single AlInN NW UV LED at 220 nm - 400 nm wavelength regime using the finite-difference time-domain (FDTD) simulations. Our results revealed that these LEDs favor transverse-magnetic (TM) polarized LEE over transverse-electric (TE) polarized emission. Further, we have explored the dependency of the LEE on the HfO_2 surface passivation layer at various layer thicknesses for ~282 nm wavelength emission. Moreover, the LEE of a single AlInN NW UV LED could be increased to ~40.6% with a 40 nm HfO_2 passivation layer from 25.2% LEE of unpassivated LED.

Simulation Setup

In this study, the LEE of the AlInN NW UV LEDs is estimated using the three-dimensional (3D) FDTD computational method (10). The AlInN NW UV LED structure grown on Si substrate is composed of 200 nm *n*-GaN, 100 nm *n*-$Al_xIn_{1-x}N$ quantum barrier (QB), 40 nm *i*-$Al_yIn_{1-y}N$ quantum well (QW), 100 nm *p*-$Al_xIn_{1-x}N$ QB, and 20 nm *p*-GaN layer. The *n*-GaN layer is tapered with a diameter from 70 nm (bottom) to 100 nm (top) on Si substrate. The diameter is set to be 100 nm for the rest of the regions. For the emission of ~282 nm wavelength, $Al_{0.78}In_{0.22}N$ and $Al_{0.825}In_{0.175}N$ are considered as QW and QB layers. To avoid the reflection of outgoing waves back to the simulation space, we have encapsulated the entire NW structure with 12 perfectly matched layer (PML) boundary conditions (11). The attenuation factor (σ) and auxiliary attenuation coefficient (κ) are set as 0.25 and 2 for this PML. For the emission of ~282 nm wavelength light, the refractive index of $Al_{0.825}In_{0.175}N$, $Al_{0.78}In_{0.22}N$, and GaN is considered 2.4132 2.4365, and 2.623, respectively (12, 13). Additionally, the absorption coefficient for the same layers taken as 70000 cm^{-1}, 79000 $cm^{-1}$and 170000 cm^{-1} in the model. We have considered the refractive index of HfO_2 to be 1.986 (14). In this study, a single TE polarized dipole source is placed in the middle of the QW to estimate the TE polarized LEE, and TE polarization is considered as the major electric field that travels in the in-plane direction [E ⊥ c-axis].

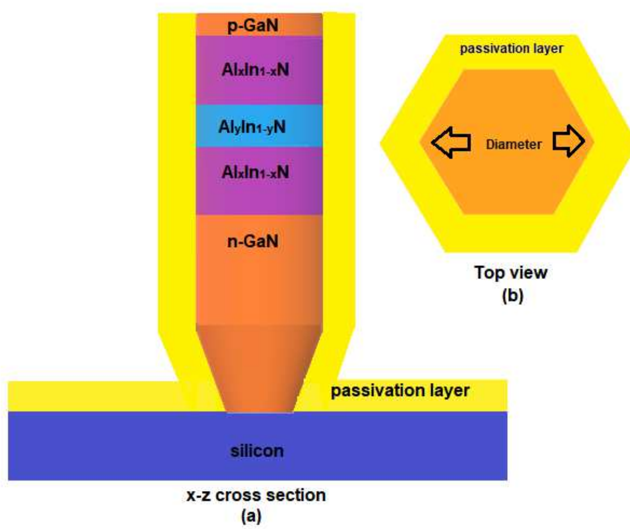

Figure 1. (a) Schematic illustration of AlInN-based NW UV LED with HfO_2 passivation layer, and (b) Cross-sectional view of NW from the top.

Similarly, TM-polarized LEE is estimated by placing a single TM polarized dipole source in the middle of the QW, and TM polarization is represented by the major electric field travels in the out-of-plane direction [E // c-axis]. Further, to measure the total power generated in the active region accurately, source power monitors are placed around the single dipole source. The total output power radiated by our NW LED is measured with the help of the output power monitors placed around the NW LED at a total distance of twice the NW diameter and an emission wavelength. Finally, we have calculated the LEE as the ratio of the light output power measured by the output power monitors to the total emitted power in the active region measured by the source power monitor. This method is commonly employed in studying the optical properties of NW structure LEDs in theoretical works (15-17).

Results and Discussion

First, we have investigated the LEE of the studied NW LED structure for wavelength ranges from 220 nm to 400 nm. Both TE and TM-polarized light sources are examined here to investigate the LEE, and the results are presented in Figure 2. It is found that the AlInN based NW structure favors TM-polarized emission, as the LEE for TM-polarized light source is consistently higher than that of the TE-polarized light source for the entire range of wavelength in the UV region. It is already established that the height of the *p*-GaN should be minimized for the reduction in absorption of the UV light (17).

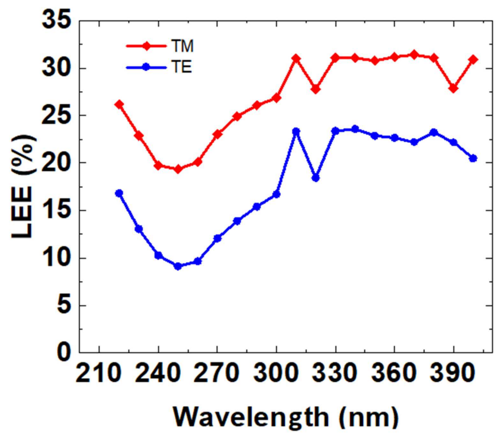

Figure 2. The LEE of the AlInN NW LED as a function of wavelength.

As shown in Figure 2, for the 282 nm wavelength, ~25.2% of LEE can be achieved for TM-polarized emission, while only ~13% of LEE is obtained for TE-polarized emission. The NW structure exhibits significantly reduced defect density and piezoelectric polarization as compared to the planar counterpart due to effective strain relaxation through the sidewalls, resulting in negligible quantum-confined Stark effect. However, due to the high surface area to volume ratio, surface density states such as dangling bonds and fermi level pinning on the NW surface are high, leading to increased non-radiative recombination near the surface (18, 19). Suppression of the surface recombination arising from these surface states can be achieved using the passivation layer. Photon trapping within the core is due to the cavity effect and must be considered while choosing NW passivation material (20). Hence, transparent material for the target range with a smaller refractive index is often used. For this study, HfO_2 was considered with an extinction coefficient (k) of 0.0045 (14). Ideally, HfO_2 with a smaller refractive index than the NW core, which is about 2.4365, in the NW should suppress the cavity effect, which traps photons and reduce the total internal reflection for all passivation layer thickness consistently. Additionally, a lower absorption coefficient should lead to more photon extraction causing higher LEE.

The dependence of LEE of AlInN NW LED for both TM and TE polarized light sources with various thicknesses of HfO_2 passivation layer ranging from 5 nm to 75nm is shown in Figure 3. The LEE due to TM-polarized light source is presented in Figure 3(a), while the LEE due to TE-polarized light source is presented in Figure 3(b). Although the critical parameters for the LEE are the refractive index and the absorption coefficient, it is understood that passivation layer thickness also has an effect on the extraction of light through the NW sidewall. As shown in Figure 3, maximum LEE of ~ 40% for TM and ~ 32% for TE polarized light can be achieved for the AlInN NW LED with an HfO_2 passivation layer of 40 nm thickness. However, for the HfO_2 layer with a lower thickness than ~ 25 nm, LEE has a decreasing trend in both TE and TM polarized light sources as the thin passivation layer properties only have a minor effect on the photons extraction. Moreover, it is seen that the LEE for the HfO_2 decreases as the thickness of the passivation layer is further increased to 75 nm thickness. This is due to enhanced total internal reflection and coupling of resonant modes between the NW core and the passivation layer. The emission of light from the sidewalls and the top surface of the AlInN NW for different HfO_2 passivation layer thickness is also studied and included in Figure 3, along with the total emitted LEE. It is found that most of the total emitted light is emitting from the sidewalls of the NWs in both the case of TE and TM polarized light sources.

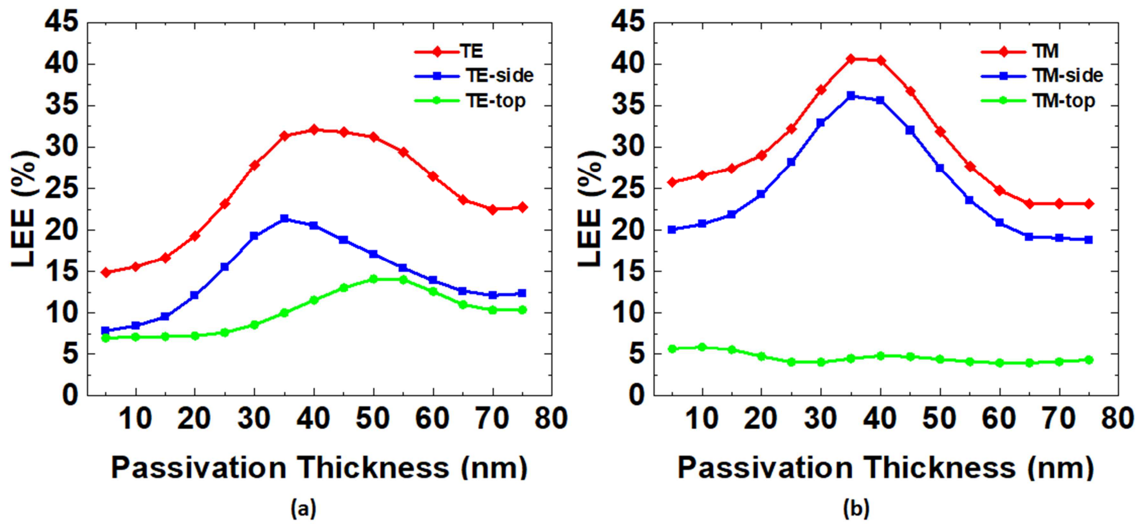

Figure 3. (a) TE-polarized, (b) TM polarized LEE of the AlInN NW LED as a function of HfO_2 passivation layer thickness.

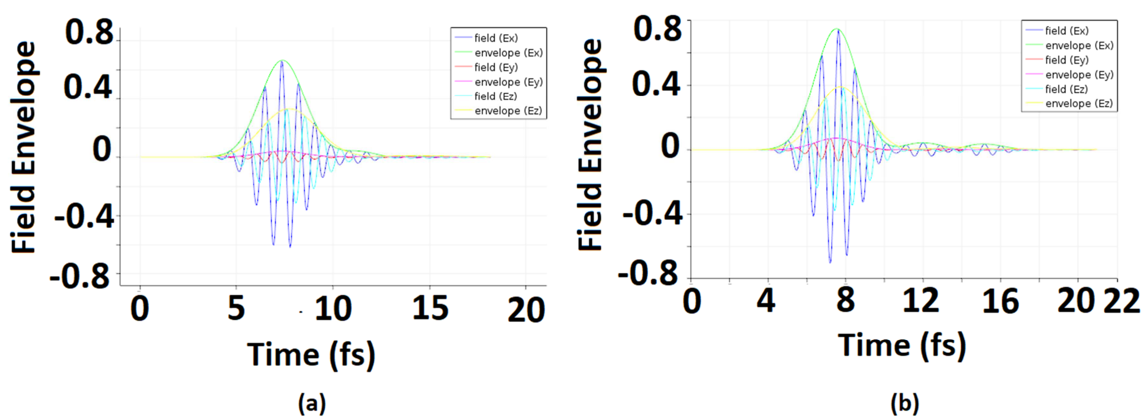

Figure 4. Electric field profile for a TM-polarized light source for a AlInN NW core in the x-y plane for (a) 40 nm thick HfO_2 passivation layer, (b) 75 nm thick HfO_2 passivation layer.

The electric field vs. time plot for the NW core with 40 nm thick and 75 nm thick HfO_2 passivation layer is exhibited in Figure 4. This figure provides information regarding the decaying of the localized resonance in the NW core. The electric field resonance plot in Figure 4 clearly shows the enhanced localized resonance in the 75 nm thick passivation layer as compared to the 40 nm passivation layer. The observed enhancement of these resonance results from increased photon confinement, paired with an increased absorption in the passivation layer; thus, the extraction efficiency of the TM-polarized light drops at 75 nm thickness, as shown in Figure 3. The absorption plots for the passivation layer of thickness 40 nm and 75 nm are shown in Figure 5. The increase in intensity certainly shows the amount of absorption, as shown in Figure 5. Because of higher confinement, and an intensive red core is seen in Figure 5b indicating more absorption in the core. Thus, increased core absorption can be attributed to more prolonged and enhanced resonance, resulting in fewer photons escaping the NW core, contributing to decreased LEE.

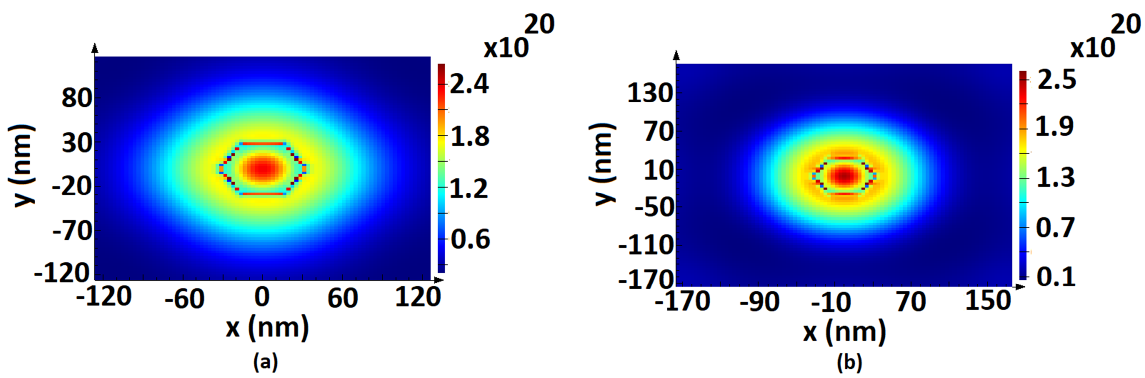

Figure 5. Cross-sectional absorption profile in the x-y plane for (a) 40 nm thick passivation layer, (b) 75 nm passivation layer.

To further understand the effect of passivation layer thickness on the TM-polarized light extraction, the electric field intensity distribution of NW LED with non-passivated, 40 nm, 75 nm thick HfO_2 passivation layer is depicted in Figure 6. As clearly illustrated in the electric field intensity plots, the TM-polarized photons, which are primarily concentrated near the active region, can easily penetrate through the NW with a thin HfO_2 passivation layer and result in large LEE. However, compared to NW with a 40 nm passivation layer, the electric field intensity is poor in the case of NW without passivation layer and NW with a 75 nm passivation layer. As thickness increases beyond 40 nm, the photons trapping along the NW core is severe due to the enhancement of resonant modes inside the thick passivation layer.

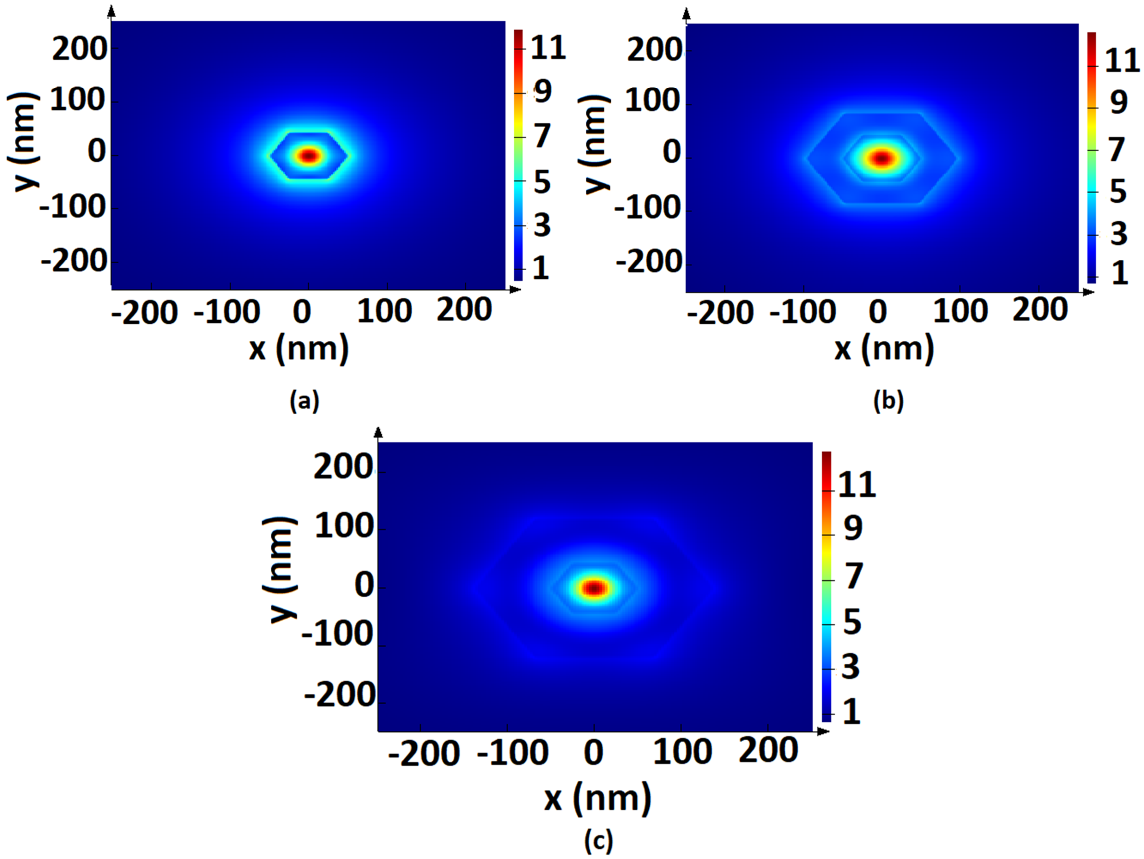

Figure 6. Cross-sectional near-field electric field intensity of a TM-polarized light source for AlInN NW LED (a) without passivation layer, (b) with 40 nm passivation layer, and (c) 75 nm passivation layer for TM-polarized light source in the x-y plane.

Conclusion

The TE/TM-polarized LEE of AlInN-based NW LED emitting across various wavelengths, and the effect of the HfO_2 passivation layer on NW for 282nm have been investigated intensively. From our analysis, a variation of LEE was observed with a different passivation layer thickness. The use of HfO_2 as a passivation layer has a smaller refractive index than the NW active region, resulting in more significant light extraction compared to NW without passivation. The maximum achievable TM and TE-polarized LEE is ~40.6% and 32% using 40 nm HfO_2 passivated structure at ~282 nm wavelength. Future work to address the impact of various photonic crystal designs within an array of NWs, such as uniformity in NW diameter, height, spacing, and peak emission wavelength, and QW position, is required to provide more comprehensive modeling of the NW LED performance.

Acknowledgments

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