Extraction efficiency simulation in deep ultraviolet AlGaIn light emitting diodes

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Extraction efficiency simulation in deep ultraviolet AlGaN light emitting diodes

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Abstract

A ray tracing model is developed to study the light extraction efficiency (LEE) of the nitride wide band gap semiconductor deep ultraviolet light emitting diodes (DUV-LEDs). The basic device structure is flip-chip LED device with dome shape encapsulation. Various device parameters such as reflecting p-metal, absorption coefficient of the AlN layer, sapphire surface roughness etc have been examined. We have found that the transparency of the AlGaN/AlN epitaxial layers as well as the encapsulation material play key roles in improving the LEE and spatial intensity distribution. To verify the transparency of the epi-layers, highly doped n-type $\text{Al}_{0.61}\text{Ga}_{0.39}\text{N}$ on AlN template are grown on sapphire substrate by high-temperature metalorganic chemical vapor deposition (HT-MOCVD), then the crystal and optical properties are measured and analyzed. The calculated the absorption coefficient of the AlN is below 10^3cm^{-1} , which paves the way to achieve high extraction efficiency DUV LEDs.

1. INTRODUCTION

Deep ultraviolet light emitting diodes, especially in the wavelength range of 260-290nm, are gaining significant attentions for research and development activities in various applications such as water purification, surface disinfection, and pharmaceutical production. Wide-band gap nitride semiconductor namely the AlGaN based multiple quantum wells (MQWs) structure in no doubt is the best candidate in achieving such short wavelength emission. Similar to nitride semiconductor LEDs in visible light spectrum range, typical DUV structures are epitaxially grown on c-plane sapphire substrate starting from thick AlN template, high Al mole-fraction n-type AlGaN current spreading layer, un-doped AlGaN MQWs, and p-type AlGaN followed with thin heavily doped p-type GaN contact layer, by MOCVD method^{[1],[2]}. Unlike the InGaN MQWs, in which microstructural features like V-pits help to prevent carriers from reaching non-radiative recombination centers so that high emission efficiency^{[3],[4]} can be obtained, DUV LEDs are much more sensitive to the presence of the epitaxial defects such as threading dislocations^{[5],[6]}. On the homoreogeneous AlN single crystal substrates with much less defects, the internal quantum efficiency (IQE) of the DUV LEDs is reported to reach as high as 70%^[7]. However, the high price and low yield of such substrate makes it hard to become popular. The AlGaN/AlN epi-layers grown on regular sapphire substrate is currently still the mainstream solution, and thus is the focus of our study.

On the other hand, device structure and fabrication processes also play important roles in improving the light extraction efficiency. For instance, the p-GaN cap layer is believed to reduce the turn-on voltage but strongly absorb DUV due to its narrower band gap. Therefore, the thickness of the top p-GaN is a tradeoff between lower contact resistance and less optical loss. Flip-chip LED structure is often used in DUV LEDs^[8], where p-contact metal has large contact area to reflect the emitted light towards substrate direction. The choosing of p-contact metal is then critical, since most of the metals are UV absorbing. Other factors, like surface roughening, encapsulation, and substrate removal etc., all affect the external quantum efficiency (EQE) of the device. They need more careful optimization compared with regular visible light LEDs. So far, the reported highest EQE of DUV LEDs can barely reach 20% with total radiated power of 100mW^[9].

In this study, we utilize ray tracing (RT) technique to analyze the dependence of light extraction behavior on various device parameters including reflection metal, existence of encapsulation layer, and the surface roughness. We developed two-dimensional simulator to solve the electromagnetic wave continuity equations in absorbing media with certain boundary conditions. Earlier reports of RT modeling on visible spectrum LEDs^{[10],[11]} can hardly be applied to DUV regime since the drastic difference in device structure. In particular, the absorption coefficient of the AlN and its alloys in DUV range is very essential to theoretical calculation but literature-inconsistent. The reported absorption coefficient of AlN thin film, which strongly depends on the deposition techniques, defects density and crystal orientations, could vary from 10^2cm^{-1} to 10^4cm^{-1} [12],[13],[14],[15]. It will result in significant difference in device performance as shown in our simulation. In order to obtain an accurate estimation, AlN grown by MOCVD at the temperature above 1300C on sapphire substrate is measured in spectrophotometer at normal incident angle. The fitted transmittance shows that the HT deposited nitride thin film has low enough absorption coefficient to achieve good light extraction in DUV LEDs.

2. MODELING

The baseline flip-chip device structure used in this study is shown in Figure 1 with reflective p-contact metal laying on the very bottom. To reduce the turn-on voltage, p-GaN cap layer above the metal is thin (10nm) enough to reduce absorption as much as possible. We assume the n-contact towards n-AlGaIn current spreading layer is done through n-via process that occupies negligible surface area. Above the cap layer, 200nm p-AlGaIn, 50nm AlGaIn/AlN MQWs, and 2000nm n-AlGaIn are stacked in sequence with Al% set to be 60%. All these device layers are grown on 3000nm thick AlN template on regular single side polished sapphire substrate, which are shown in Figure 1 as the top two layers within the encapsulation. Although nano-pattern sapphire substrate (NPSS) is reported to enhance the crystal qualities during AlN template growth^[16], we didn't take it into account because those wavelength-comparable sized patterns and consequently the lateral overgrowth induced hollow cavities at AlN/sapphire interface will bring in complicated scattering effects that need electromagnetic wave simulation and make the RT calculation almost impossible.

Also we assume the sapphire substrate is thinned down to $50\mu\text{m}$. Usually the after-lapping, sapphire surface roughness ranges from 0.5 to $2\mu\text{m}$, which is much larger than the wavelength of DUV. Quite some theoretical calculations were done to study the scattering effects on the rough surface by solving Maxwell's equations to predict the propagation of

light waves^{[17],[18]}. It shows that both the reflection and the refraction light should be treated with diffusive and specular components. Usually, those numerical calculations can hardly be implemented in RT models due to heavy computational complexity. Instead, empirical models based on bidirectional scattering distribute function (BSDF) to describe rough surface consists of microfacets are widely adopted in RT calculations. They have been intensively studied by Phong, C-T, O-N and GCX ^{[19],[20],[21],[22]}, and successfully applied in the area such as computer image/graphic rendering. As illustrated in Figure 2(a), we here assume the reflection and refraction light scattered at the rough interface follows Gaussian distribution, and the surface microfacets distribution follows Beckmann function (Equation 1), where θ_m is the angle between incoming ray and marco-surface normal direction.

$$D = \frac{1}{\pi \alpha_b^2 \cos^4 \theta_m} \exp\left(-\frac{\tan^2 \theta_m}{\alpha_b^2}\right) \quad (1)$$

Take refraction light for example, Figure 2 (b) shows calculated transmittance function (solid line). The dashed lines represented the angular distribution of the transmittance for the light rays at 10-, 30- and 50-degree incident angle. For simplicity, we consider the diffusive lights from surface scattering as the second light source with limited angular sampling, and omit any re-entrance back into sapphire bulk.

Encapsulation packaging between device and air is very useful in LEDs industry to improve light extraction efficiency. On the other hand, DUV transparent encapsulation material is not mature yet because of the absorption from organic compounds. Quartz or sapphire based inorganic encapsulation although has no worry on transparency, but its poor resistance to air moisture and difficulties in processing are still main obstacles. Alternatively, DUV transparent organic compounds such as methyl-siloxane, fluorinated resin ^{[23], [33]} are compatible with current LEDs process. In our baseline structure, we still assume a 250 μ m thick (radius) dome shape encapsulation is applied.

Most of the metals participating in good ohmic contact formation in regular LEDs process are not suitable in DUV spectrum range due to strong absorption. The possible candidates are Al, W, Rh ^{[24],[25],[26]}, but there are no experimental evidences showing that they alone could produce reasonably low contact resistance to p-GaN. Therefore, thin Ni(2nm) is laid first as contact layer, then caped with those reflecting metal, together to form the p-contact. Three cases namely Ni/W, Ni/Rh and Ni/Al are examined and compared. The calculated s-polarization and p-polarization reflectance on those bi-layer stacks are plotted in Figure 3. Theoretically Al could provide highest reflectance in DUV, therefore Ni/Al stack is considered as the baseline option. In all, the main device parameters used in this modeling are summarized in Table 1, noting that the optical properties are given at 280nm wavelength.

3. RESULTS AND DISCUSSIONS

Figure 4 (a) shows the distribution of the light rays plot from: baseline structure; baseline without encapsulation; baseline without encapsulation plus the sapphire top surface is ideally smooth. The simulation is assuming the light rays originated from the MWQs are identical towards every direction. As we can see the trapping of the light rays inside the chip especially in nitride films is still obvious. In ideal cubic geometry, most of the light will be reflected back and forth between interfaces. The dome shape encapsulation on the other hand could help light rays reaching its boundary to get extracted. Since many materials are lossy in this structure, usually after approximately 10 times bouncing between interfaces, the rays will vanish (below 10% of the original intensity). The rough surface of top sapphire acts

as diffuser to randomize the propagation. Here the LEE is defined as the intensity ratio between output rays traveling into air and the rays generated in the MQWs, and value comes out to be 35.5% for the baseline structure. Figure 4(b) shows the angular intensity distribution for the LEDs in all these three configurations. The dome shape encapsulation significantly improves the extraction of the light by widening the emission range from ± 60 degree to almost ± 90 . The existence of the surface roughness, on the other hand, helps to make the distribution within emission angle more uniform.

Table 2 listed the calculated LEE of the devices with various configurations at 280nm wavelength. Encapsulation is the most effective way to reduce the TIR effect and get more lights out of the chip, as the LEE increases more than 10% from the one without encapsulation. Top surface roughness is the second biggest factor on improvement. Compared with the reports on conventional visible light LEDs [27], this increment is not that significant. Possible reasons may include the absorption from the p-contact; ideally smooth chip edge; and non-lambertian scattering from sapphire surface. Different p-metal stack, on the other hand, has small influence (less than 2%) on the LEE compared to the baseline device structure. Obviously, if highly absorbing p-GaN is eliminated from the LEDs, significant improvement can be expected.

We found the absorption coefficient of the AlGaIn/AlN epi-layers and the encapsulation material, plays important role in determine the output ray intensity. For instance, the LEE of the baseline structure drops approximately 4% if the absorption coefficient of the AlN increase from 10^2 cm^{-1} to 10^3 cm^{-1} , and the efficiency will reduce down to single digit if the coefficient reaches 10^4 cm^{-1} . The encapsulation's absorption has even greater impact, due to much larger traveling distance before the rays leave it. The relationship between LEE and encapsulation thickness (dome radius) under different absorption coefficients is plotted in Figure 5. As we calculated, the threshold values for absorption coefficient (at $250 \mu\text{m}$ thickness) and thickness (at 10 cm^{-1} absorption coefficient) of the encapsulation are 23 cm^{-1} and $491.8 \mu\text{m}$ respectively, which means the LEE will benefit no more from encapsulation if its absorption or thickness is greater than that number.

One important phenomenon observed on nitride LEDs is the polarized emission. It is found that the in-plane (c-plane) light emitted from AlGaIn based MQWs switches its polarization characteristic from transverse electric (TE) to transverse magnetic (TM) mode at some critical Aluminum composition[28]. Such transition is caused by the strong build-in strain that could split the valance band of the nitride into heavy hole and split-off hole sub-bands[29]. If the lowest energy excitation in MQWs is a heavy hole, then TE polarization is obtained, otherwise it will be TM mode. The degree of the polarization, defined as $P = (I_{TE} - I_{TM}) / (I_{TE} + I_{TM})$, for 280nm DUV LEDs is reported around -0.1 if grown on sapphire substrate[30]. Hereby, we also take polarization into account in our modeling. The LEE calculated in Table 2 is assuming zero degree of polarization. While in case of TM polarized emission ($P = -0.1$), the LEE drops slightly by 1.4% which is not as significantly as other literature[31]. The RT model presented here assumes the degree of elliptic polarization from MQWs emission has uniform spatial distribution along every direction. If the emission from the MQWs can be restored to TE mode, then the performance of the device can be improved. The fine tune on barrier Al composition and film stress could be the way to achieve it.

To evaluate the properties of the high Al-content nitride epi-layer, we specially optimize

the growth conditions of AlGa_N and AlN films on planar 2-inch sapphire substrate using high temperature (over 1300C) MOCVD tool. Trimethylaluminum (TMAI) and NH₃ are Al and N sources respectively. High quality crack-free thick AlN film was obtained after optimizing the growth conditions. The thickness non-uniformity of 3μm thick AlN template is below 2%, with 157 and 358 arcsec full width half maximum (FWHM) on (002) and (102) orientations measured in X-ray diffraction (XRD) shown in Figure 6. Highly doped n-type AlGa_N film deposited on such AlN template was also achieved, with Al mole fraction reaching 61% by XRD. The sheet resistance of the n-AlGa_N film reaches 1370 Ω/□ identified by room temperature hall measurement. The wafer warpage of the 2 inch sapphire is below 20μm indicating a good stress control during the growth.

The transparency of our HT MOCVD grown AlN on double side deposited sapphire is studied. The transmittance of the film is measured in LAMBDA 750 UV-NIR spectrophotometer. The solid line in Figure 7 is the transmittance of this sample in the wavelength from 200 to 550nm with normal incidence. The interference oscillations in visible light spectrum range helps to identify the film thickness. We assume the absorption coefficient of the MOCVD grown AlN follows exponential distribution^[32] over the wavelength as following

$$\alpha = A \cdot \exp(B \cdot \lambda) \quad (2)$$

where A and B are the factors to be fitted. The coefficient of the AlN is then calculated to be 10^{2.2} cm⁻¹, and the simulated transmittance is plotted in dotted line in Figure 7 which matches well with the measurement. Experimentally, we are now running epi-condition optimizations for the active region within DUV LEDs. For further improvement on light extraction, TE polarized emission study and the optical properties of the fluorine resin encapsulation are our main focus.

4. CONCLUSIONS

Ray tracing modeling is applied to the high Al% concentration nitride semiconductor LEDs aiming on 280nm wavelength emission. The baseline device structure used in this study has flip chip configuration with high reflective NiAl p-metal contact; thin p-GaN contact layer; roughened top sapphire surface and dome shape low loss encapsulation material. We found the light extraction efficiency could reach 35.5% with spatial distribution covers nearly entire upper sphere. As comparison, without encapsulation, the efficiency drops more than 10% and the emission angle narrows to ±60 degree. Surface roughness also helps in enhancing LEE and uniformly distributing the light. Due to the existence of the absorbing p-GaN, different p-metal stacks bring less influence on LEE. Absorption coefficients of both nitride semiconductor and encapsulation play important roles. To achieve reasonably good LEE, the absorption coefficients of nitride and encapsulation should be kept below 10³ and 20 cm⁻¹ respectively. Furthermore, high temperature AlN and n-Al_{0.61}Ga_{0.39}N films are epitaxially deposited on planar sapphire substrate and evaluated with XRD, Hall and spectrophotometer measurements. The fitting shows the absorption coefficient of our MOCVD deposited nitride film is around 10^{2.2} cm⁻¹ at 280nm wavelength which is suitable the DUV LEDs process.

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TABLES AND CAPTIONS

<i>Layers</i>	<i>Parameters</i>
p-metal	$W=200\mu\text{m}$, $\text{Ni}=2\text{nm}$, $n=2.02$, $\kappa=2.24$
p-GaN cap	$d=5\text{nm}$, $\alpha=1.6\text{e}+5\text{ cm}^{-1}$, $n=2.58$
p-AlGaIn	$d=200\text{nm}$, $\text{Al}\% =60\%$, $\alpha=1.0\text{e}+3\text{ cm}^{-1}$, $n=2.29$
MQWs	$d=50\text{nm}$, $\alpha=1.0\text{e}+3\text{ cm}^{-1}$,
n-AlGaIn	$d=2000\text{nm}$, $\text{Al}\% =60\%$, $\alpha=1.0\text{e}+2\text{ cm}^{-1}$, $n=2.29$
AlN buffer	$d=3000\text{nm}$, $\alpha=1.0\text{e}+2\text{ cm}^{-1}$, $n=2.1$
Sapphire	$d=50\mu\text{m}$, $n=1.82$, $\alpha_b = 0.6$
Encapsulation	$R=250\mu\text{m}$, $n=1.45$, $\alpha=1.0\text{e}+1\text{ cm}^{-1}$

Table 1: LED device parameters used in this study, where d denotes for layer thickness, W is the device width and R is the radius of the encapsulation, n , κ , α are refraction index, extinction and absorption coefficient respectively at 280nm wavelength.

<i>Configurations</i>	<i>LEE</i>
Baseline structure (p-metal is NiAl)	35.5%
Baseline but without encapsulation	22.9%
No encapsulation, smooth sapphire	19.1%
Baseline but p-metal is NiRh	34.9%
Baseline but p-metal is NiW	35.1%

Table 2: Calculated LEE with various DUV LED configurations at 280nm wavelength.

FIGURES AND CAPTIONS

Figure 1: Baseline device structure used in this study

(a)

(b)

Figure 2: (a) Illustration on the specular and diffusive components for the lights refracted and reflected at rough sapphire interface. (b) The calculated transmittance (solid line) at the rough sapphire/encapsulation interface, with angular distributions for incoming angle at 10, 30 and 50 degree (circle, plus and dot marks respectively).

Figure 3: Calculated s-polarized and p-polarized incident light (at 280nm) reflectance on Ni/Al, Ni/W and Ni/Rh metal stacks, with Ni thickness is 2nm.

(a)

Figure 4: (a) Light ray plot for the UV LED with dome shape encapsulation. (b) Angular light intensity distribution for the UV LED in different configurations (with or without sapphire roughening, with or without encapsulation)

Figure 5: The dependency of LEE on the radius of dome encapsulation, with different absorption coefficients.

Figure 6: (a) Thickness mapping showing thick ($>3\mu\text{m}$) uniform AlN template layer grown on 2 inch planar c-sapphire. (b), (c) FWHM of the AlN layer on (002) and (102) orientations by XRD measurement.

Figure 7: The as-measured and simulated transmittance of the 320nm thick MOCVD grown AlN layer on double-sided polished sapphire substrate. The absorption coefficient of the AlN film is $10^{2.2} \text{ cm}^{-1}$ at 280nm wavelength.

Figures

Figure 1

Baseline device structure used in this study

(a)

(b)

Figure 2

(a) Illustration on the specular and diffusive components for the lights refracted and reflected at rough sapphire interface. (b) The calculated transmittance (solid line) at the rough sapphire/encapsulation interface, with angular distributions for incoming angle at 10, 30 and 50 degree (circle, plus and dot marks respectively).

Figure 3

Calculated s-polarized and p-polarized incident light (at 280nm) reflectance on Ni/Al, Ni/W and Ni/Rh metal stacks, with Ni thickness is 2nm.

(a)

Figure 4

(a) Light ray plot for the UV LED with dome shape encapsulation. (b) Angular light intensity distribution for the UV LED in different configurations (with or without sapphire roughening, with or without encapsulation)

Figure 5

The dependency of LEE on the radius of dome encapsulation, with different absorption coefficients.

Figure 6

(a) Thickness mapping showing thick ($>3\mu\text{m}$) uniform AlN template layer grown on 2 inch planar c-sapphire. (b) , (c) FWHM of the AlN layer on (002) and (102) orientations by XRD measurement.

Figure 7

The as-measured and simulated transmittance of the 320nm thick MOCVD grown AlN layer on double-sided polished sapphire substrate. The absorption coefficient of the AlN film is 102.2 cm^{-1} at 280nm wavelength.