Influence of the microstructure geometry of patterned sapphire substrates on the light extraction efficiency of GaN LEDs

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The influence of the microstructure geometry of patterned sapphire substrates (PSS) on the light extraction efficiency (LEE) of GaN light-emitting diodes (LEDs) is numerically analyzed. Cone structures of various dimensions are studied, along with dome and mixed microstructures. LEE is found to mainly depend on the microstructure surface slope. LEE rises quickly with slope and flattens out when the slope exceeds 0.6. Scaling down the microstructure has little effect on LEE. Light rays are found to travel longer distances in PSS LEDs, as compared with LEDs grown on a flat substrate. Keeping GaN absorption loss low is important for LEE optimization.

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1. INTRODUCTION

GaN light-emitting diodes (LEDs) have attracted considerable attention due to their promising potential in general lighting applications. GaN has a fairly small total internal reflection angle due to its high refractive index. As a result, most of the light emitted in a planar device structure is trapped inside GaN, resulting in a low LEE value. Many attempts have been made to improve the LEE, including applying different textures on the front LED or back sapphire surfaces [1–4] and using various micro/nanostructure PSS [5–13]. Current high-brightness LEDs are mostly grown on PSS, which has arrays of 3D patterns on its surface, often a pyramidal shape array. The 3D pattern increases LEE by scattering the trapped light rays into different directions outside the total internal reflection angle. Besides increasing LEE, PSS can also reduce GaN defect density due to the forced lateral growth by the 3D pattern [14–17], which can lead to better internal quantum efficiency. The effect of PSS pattern geometry on LEE is a critical issue and informs PSS design optimization. LEE values of 80% have been reported in a carefully optimized device [18]. Numerical analysis has been used to study LEE enhancement through different surface textures and patterns [19–23]. However, systematic comparisons among different pattern geometric parameters (e.g., height, spacing, and size) and comparisons of different pattern shapes are still lacking. Here, we report a numerical study on these variables and identify the important dimensions in PSS pattern design. In the analysis, we also consider cases with and without material absorption loss. We obtain an average light ray propagation path length inside the PSS GaN LED before breaking total internal reflection. The obtained long path length indicates that GaN absorption loss is also an important factor to consider for LEE optimization.

2. STRUCTURE MODEL

Three-dimensional patterns on PSS can assume different shapes, including cones, domes, pyramids, and cylinders. They are often organized in different array patterns. Some basic dimensions for the width, height, and spacing of 3D patterns are widely used, with the most commonly used dimensions being around 1–2 μm in width, 1–2 μm in height, and sub μm in spacing. In this paper, we use the Monte Carlo ray tracing method to analyze the LEEs of PSS LEDs with different dimensions. The software tool TracePro is used for calculations. The schematic of the simulation model is shown in Fig. 1(a). The layer thickness structure consists of a 150 μm sapphire, a 4.5 μm n-GaN, a 125 nm InGaN/GaN multiple quantum well (MQW), and a 230 nm p-GaN. The chip size is 50 μm × 50 μm. Different chip sizes at 75, 100, and 200 μm...
3. SIMULATION RESULTS AND DISCUSSION

We first calculated the changes of LEE as the cone height \((h)\) varies from 0 to 3.2 \(\mu\text{m}\), while the width \((w)\) and spacing \((s)\) were respectively fixed at \((w,s) = (2.6, 0.4) \mu\text{m}\). We considered three material scenarios: GaN without absorption (GaN), GaN with absorption (GaN/abs), and GaN with absorption and a 98% reflective Ag coating at the backside of the sapphire (GaN/abs/Ag). The without absorption loss case is to provide an ideal upper bound LEE value. In practice, there is always some material loss that gives lower LEE value. The cone-height-dependent LEE values are shown in Fig. 2(a). The LEE at a cone height of 0 \(\mu\text{m}\) is basically the LEE of a conventional planar LED. The value is only 31.7\%, indicating that a large portion of light rays are trapped by total internal reflection. As the cone height increases to 0.8 \(\mu\text{m}\), the LEE of the PSS LED quickly increases to 89.1\% and reaches a maximum of 91.3\% at a cone height of 1.6 \(\mu\text{m}\) and then slightly decreases to 88.7\% as the cone height further increases to 3.2 \(\mu\text{m}\) [solid blue line in Fig. 2(a)]. We have also calculated the LEE curve for different \((w,s)\) at \((2.6, 2.0) \mu\text{m}\) (dotted blue line). It is lower than the \((w,s) = (2.6, 0.4) \mu\text{m}\) case (solid blue line). However, it still shows a similar fast rise followed by a plateau. This indicates that the characteristic of the dependence of LEE on height is fairly independent of the spacing parameter.

We then included the material absorption loss in a calculation with \((w,s) = (2.6, 0.4) \mu\text{m}\). The LEE of the planar GaN/abs LED decreases slightly from 31.7\% to 29.5\%. As the cone height increases, the LEE of GaN/abs PSS LED has a similar fast rise and flattening behavior [red line in Fig. 2(a)]. However, the LEEs are much lower due to material loss. GaN absorption does not alter the light ray propagation path. Those light rays escaping total internal reflection still go through the same multiple reflection routes and experience GaN absorption loss while propagating inside GaN. The LEE can be expressed as

\[
\text{LEEP} = \frac{1}{P_i} \sum_{i=1}^{n} P_i \exp(-\alpha X_i) \cong \frac{1}{P} \sum_{i=1}^{n} P_i \exp(-\alpha L),
\]

where \(P_i\) is the power of the escaped light ray in free space when there is no absorption loss, i.e., \(\alpha = 0\). The light ray is assumed to have traveled \(l_i\) path length in GaN. When the absorption loss is considered, the escaped light ray power is \(P_i\) multiplied by an absorption loss \(\exp(-\alpha X_i)\). \(P\) is the original total power emitted from MQWs. We introduce an averaged path length \(L\) in the second equality. \(L\) is basically obtained by averaging the loss term \(\exp(-\alpha l_i)\) weighted by power \(P_i\). The LEE with material absorption loss is equivalent to the LEE without absorption loss multiplied by the averaged path length loss \(\exp(-\alpha L)\). For planar LED \((b = 0)\), the LEE decreases from 31.7\% to 29.5\% when GaN absorption loss is included. The averaged loss path length \(L\) calculated from 29.5\% = 31.7\% \times e^{-8.5} is 9 \(\mu\text{m}\), where GaN absorption \(\alpha = 8 \text{ mm}^{-1}\) is used. The averaged loss path length \(L\) versus cone height, obtained by a similar calculation, is shown in Fig. 2(b). When cone height increases slightly to 0.2 \(\mu\text{m}\), the average loss path length in GaN jumps to 49 \(\mu\text{m}\). This sudden increase is caused by some of the originally trapped light rays being able to break total internal reflection. Their path lengths change from infinite loops inside GaN to finite but are still fairly long paths in GaN, as compared with the GaN layer thickness. These light rays contribute to the significant increase of the averaged light
ray propagation path length $L$. The loss path length gradually decreases to 35 μm as cone height increases and levels off at 2.6 μm. The average propagation path length in PSS LEDs is much longer than that in planar LEDs, indicating that light rays reflect off the cone surfaces many times to escape from the total internal reflection. Keeping material loss low is therefore important for PSS LEDs. Finally, when an Ag reflector is introduced on the sapphire backside, the LEEs of GaN/abs/Ag PSS LEDs lose an additional 2%–9% [difference from the red to green line in Fig. 2(a)] even though Ag loss is only 2%. The additional loss is due to the repeated propagation through GaN when light rays are reflected off Ag.

We then fixed $(w, h)$ at (2.6, 1.6) μm and varied the cone spacing from 0 to 2.6 μm. The calculated LEE values are shown in Fig. 3(a). Without considering loss, the LEE (blue line) stays around 91% for spacing from 0 to 0.5 μm and then decreases to 83.6% when spacing increases to 2.6 μm. The decrease in LEE is due to the large spacing producing a greater flat surface, which cannot change the diverted light rays out of the trapped directions. It is worth noting that reducing cone spacing below 0.4 μm has little effect on LEE. This is likely because once the flat surface region is small enough, light rays are likely to be scattered by the cone surfaces out of total internal reflection. We have also calculated the LEE curve for $(w, h) = (2.6, 0.4) \mu m$ (dotted blue line). It is lower than the $(w, h) = (2.6, 1.6) \mu m$ case (solid blue line). The decreasing characteristic is similar. The behavior of the dotted and solid blue lines in Figs. 2(a) and 3(a) indicate that the behavior of the LEE curve versus either height or width is fairly independent of the values of the other two fixed parameters. When GaN absorption loss is considered, LEE (red line) is much lower compared with the no absorption case (blue line). The averaged loss path length can be calculated from the ratio between with loss and without loss values as described previously [Fig. 3(b)]. The average path length increases with cone spacing because the larger flat surface spacing causes light rays to traverse a much longer distance to break off total internal reflection.

We next considered scaling the cone size. We used $(w, s) = (2.6, 0.4) \mu m$ and heights from 0 to 3.2 μm as references and scaled down all dimensions proportionally by 1/2 and 1/4. Cone width values of 2.6, 1.3, and 0.65 μm were respectively used to label PSS 2.6, PSS 1.3, and PSS 0.65. From the GaN refractive index, the effective wavelength inside a commonly used 450 nm LED is 187 nm. This is still smaller than 0.65 μm. We therefore assume that the ray tracing method still provides valid estimates. The calculated LEE curves without GaN absorption loss are shown in Fig. 4(a). The maximum LEEs are respectively 91.3%, 92.3%, and 91.9%. The maximum values are fairly close but occur at different cone heights. When we plot the curves versus the surface slope defined by $2h/w$, as shown in Fig. 4(b), the three curves are almost converged. The LEE curves with GaN absorption loss are shown in Fig. 4(c). The LEE versus surface slope is shown in Fig. 4(d). The LEE curves are fairly close. The analysis shows that LEE is mainly determined by the surface slope rather than the pattern size. Scaling down the cone size does not change the LEE curve much. The LEE curve generally has a fast rise as the surface slope increases and saturates at a surface slope of around 0.6 without material absorption loss. The saturation point moves to a larger slope value of ~1.2 when absorption loss is present. The great similarity of LEE curves when plotted versus surface slope indicates that the surface slope of the cone pattern is an important factor affecting LEE.

So far, we have only considered cone-shaped PSS. We now use a dome shape to study the shape effect on LEE. For comparison, we use the same fixed $(w, s) = (2.6, 0.4) \mu m$ and calculate LEE versus height from 0 to 3.2 μm. The dome shape is
an ellipsoid with height and width as its major and minor radii, respectively. The calculated LEE for GaN and GaN/abs PSS LEDs are shown in Fig. 5. The LEE values for cone-shaped PSS LEDs are also included for comparison. The dome-shaped LEE performs slightly better than the cone-shaped LEE up to a height of 1.2 μm without absorption loss. When absorption loss is considered, its LEE is better up to a height of 1.6 μm. If we compare the maximum LEE values of these two patterns, the difference is only 1%. They are not significantly different. We further study various PSS shapes, as shown in Figs. 6(a)–6(f), including cone, concave, cylinder, convex (dome), 2-step cone, and mixed cone and dome shapes. The sizes are all fixed at 2.6 μm width, 0.4 μm spacing, and 1.6 μm height. The LEEs of each shape are shown in Fig. 6(g) for GaN without absorption loss (GaN) and with absorption loss (GaN/abs). The values are all fairly close except for the cylinder shape either with or without GaN absorption loss. The much lower LEE for the cylinder pattern is due to its horizontal and vertical surface angles being the same as the original rectangle surface angles and thus cannot help to redirect the trapped light rays out of the total internal reflection angle. With this exception, the very similar LEEs of these different patterns indicate that the inclined surface slope variations have a large tolerance window for breaking total internal reflection, and the details of the geometrical shape do not have a critical impact.

4. SUMMARY

We have studied the influence of various pattern geometries on the LEE of PSS GaN LEDs. LEE increases quickly as cone height increases from zero and flattens out when the cone surface slope reaches 0.6. The cone spacing should be kept small in the sub μm range to reduce the flat surface area. We obtained an averaged light ray propagation path length in GaN by analyzing the LEEs with and without GaN absorption loss. The use of PSS can greatly increase the LEE at the expense of significantly increasing the overall light ray propagation path length in GaN. It is therefore important to keep material loss low for LEE optimization. The scaled down PSS pattern gives similar LEE values. LEE is mainly determined by the patterned surface slope. Dome and various mixed shape PSS with similar sizes all show similar LEE values, except the cylinder shape. This indicates that the inclined surface is important in increasing LEE and can have a large operation window.

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Fig. 6. (a)–(f) Various PSS patterns for 2.6 μm width, 0.4 μm spacing, and 1.6 μm height. (g) LEEs of patterns (a)–(f) for GaN without absorption loss (GaN) and with absorption loss (GaN/abs).