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Hole Injection and EBL Structure Optimization in GaN Micro-LEDs based on Silvaco TCAD

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Abstract

As Micro-LED display technology advances toward higher resolution, higher brightness, and higher current density, the effects of device scaling on carrier transport and interfacial behavior become increasingly significant. In GaN-based Micro-LEDs, the distinct effective masses, mobilities, and transport characteristics of electrons and holes generally result in weaker hole injection, which can lead to nonuniform carrier distribution in the active region and thereby limit radiative recombination in the quantum wells. Although the electron blocking layer (EBL) can suppress electron overflow toward the p-GaN side, its thickness and acceptor doping conditions also affect hole transport into the multiple-quantum-well (MQW) region. Therefore, the EBL structure and p-GaN doping require further optimization. In this work, a two-dimensional GaN/InGaN MQW Micro-LED device model was established using Silvaco TCAD. A self-consistent drift-diffusion transport model was employed to analyze the internal band structure, hole quasi-Fermi level, and hole current density. The results provide a two-dimensional TCAD-based approach for the optimization of EBL and p-GaN structural parameters in GaN-based Micro-LEDs.

Keywords

Micro-LED; Silvaco TCAD; Electron Blocking Layer; Hole Injection; Two-Dimensional Device Simulation.

1. Introduction

Micro-LEDs offer high brightness, high contrast, fast response, and long lifetime, making them promising for high-resolution display applications[1,2]. As the device dimensions continue to shrink, carrier transport within the device becomes increasingly important to the luminescence performance[3]. For GaN-based micro-light-emitting diodes, the low hole mobility in p-GaN and the limited activation efficiency of Mg acceptors hinder the injection of holes into the InGaN multiple quantum well region[4]. This situation is likely to cause uneven distribution of carriers in the active region, which in turn affects the recombination process of carriers[5,6].

In GaN-based LEDs, the electron blocking layer (EBL) is usually placed between the multi-quantum well (MQW) active region and the p-type GaN layer. Its main role is to reduce electron leakage into the p-GaN side and to strengthen carrier confinement within the active zone. An AlGaN EBL improves electron confinement by raising the conduction band offset, but a higher barrier can simultaneously impede hole transport. Hence, when designing the EBL, both electron suppression and hole injection into the MQW must be taken into account. Specifically, the EBL thickness as well as Mg doping levels in the p-GaN and the EBL influence the internal energy-band profile and spatial distribution of carriers.

Current optimization studies of EBLs in GaN-based LEDs mainly focus on material composition, thickness, and doping conditions, while the effects of these parameters on hole transport require

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further investigation. For Micro-LEDs in particular, external current alone cannot directly reveal the hole transport behavior within the MQW region. Therefore, internal physical quantities such as the band structure, hole quasi-Fermi level, and hole current density should be considered.

In this work, a two-dimensional GaN/InGaN MQW Micro-LED model was established using Silvaco TCAD to investigate the effects of EBL thickness, p-GaN doping concentration, and EBL Mg doping concentration on hole transport. Based on parameter screening, suitable structural parameters were identified, and the optimized structure was further compared with the baseline structure to evaluate the influence of EBL-related parameters on hole injection into the quantum-well region. This study provides a numerical reference for EBL design and hole-injection optimization in GaN-based Micro-LEDs.

2. Simulation and Device Structure

2.1 Working Principle of GaN-based Micro-LED

A typical GaN-based micro-LED consists of an n-GaN layer, InGaN/GaN multiple quantum wells (MQWs), and a p-GaN layer as the fundamental light-emitting structure[7]. Under forward bias, electrons flow from the n-GaN side, while holes are supplied from the p-GaN side. These injected carriers recombine inside the InGaN/GaN MQW region and emit photons. Therefore, efficient carrier injection and confinement within the MQW region are essential for micro-LED performance.

In GaN-based devices, electron and hole transport behaviors differ considerably. Owing to the comparatively low hole mobility and the limited ionization of Mg acceptors, which restricts the hole concentration in p-GaN, injecting holes from p-GaN into the MQW region becomes relatively difficult. Accordingly, device design must not only reduce electron overflow toward the p-GaN side but also ensure adequate hole injection into the active region.

2.2 EBL Structure and Hole Injection

In a typical LED structure, the electron blocking layer (EBL) is positioned between the multiple quantum well (MQW) active region and the p-GaN layer. Its primary purpose is to raise the potential barrier for electrons traveling from the MQW toward the p-GaN side, thus limiting electron leakage and enhancing carrier confinement in the active zone. In the present work, an AlGaN layer was employed as the EBL.

However, because this layer lies between p-GaN and the MQW region, its structural characteristics influence both electron flow and hole transport toward the quantum wells. For instance, variations in EBL thickness and doping profiles alter the internal energy-band alignment and the way carriers move. If the transport barrier becomes too high, hole injection into the MQW can be impeded, whereas a suitably lowered barrier tends to promote hole injection.

Given these factors, this study emphasizes hole transport into the MQW region instead of focusing only on electron-blocking performance. Accordingly, the EBL thickness, the p-GaN doping level, and the Mg doping concentration in the EBL were adjusted to optimize device performance.

2.3 Two-dimensional Device Structure

To investigate the effects of the above structural parameters on hole transport, a two-dimensional GaN-based Micro-LED device model was established using Silvaco TCAD, as shown in **Fig. 1**. The vertical device structure consists of n-GaN, InGaN/GaN MQWs, an AlGaN EBL, and p-GaN[8,9].

Five periods of InGaN/GaN MQWs were employed as the active region, with an In composition of 0.20 in the InGaN wells. In the device model, the top boundary of the MQW region was fixed at y=0.927 μm, which served as the common reference position for the EBL and upper p-GaN structure. In the baseline structure, the AlGaN EBL thickness was 15 nm, the Al composition was 0.15, the EBL Mg doping concentration was $2\times10^{18}cm^{-3}$, and the p-GaN doping concentration was $1\times10^{19}cm^{-3}$.

In the parameter sweep, the thickness of the EBL, the doping level of p-GaN, and the Mg doping concentration within the EBL were each changed separately so that hole transport behavior could be

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compared across different structural configurations. Section 3 presents the specific ranges of these parameters and the resulting optimized structure.

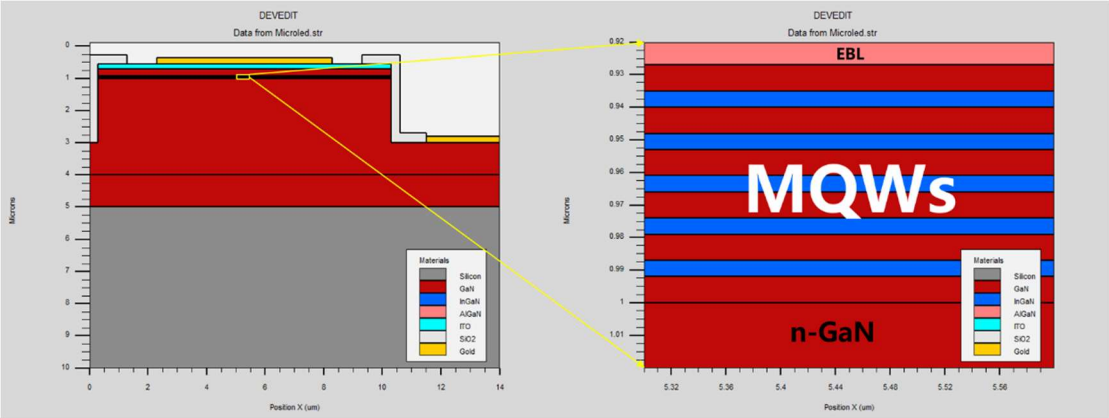

Fig. 1 Micro-LED cross-sectional structure and quantum well layer distribution

2.4 Simulation Conditions

The two-dimensional Micro-LED device was simulated using Silvaco ATLAS. Polarization and strain-related effects were included, while Fermi statistics and Shockley–Read–Hall (SRH) recombination were employed to describe carrier behavior within the device. The work functions of the anode and cathode were set to 5.3 and 4.3 eV, respectively.

Based on the objectives of the analysis, specific bias points were chosen to examine the internal energy-band structure and carrier transport behavior. The main extracted quantities included the hole quasi-Fermi level, valence-band energy, and hole current density (Jh). Among these quantities, the hole current density was used as the primary indicator of hole transport into the MQW region.

Because numerical convergence was limited under some high-bias conditions, the analysis mainly used bias points at which reliable structure solutions could be obtained. Incomplete I–V sweeps were therefore not used as the primary evaluation criterion.

3. Results and Discussion

3.1 Effect of EBL Thickness on Hole Transport

EBL thickness is an important structural parameter affecting hole transport from p-GaN to the MQW region. To investigate its influence, device structures with EBL thicknesses of 10, 15, and 20 nm were simulated, and the hole quasi-Fermi level, valence-band energy, and hole current density were extracted from the available reliable solutions. The comparison of hole current density for device structures with three different EBL thicknesses is shown in **Fig. 2** (a).

For the 10-nm EBL structure, numerical convergence was limited at higher bias. Therefore, the corresponding structure file from the 1.00-V target solve could not be regarded as a true 1.00-V solution. In contrast, reliable solutions could be obtained at lower bias. At a forward bias of 0.30 V, the hole quasi-Fermi level near the EBL/MQW interface stayed close to 0 eV, while it changed noticeably after moving into the MQW region, indicating that the applied voltage modified the distribution of hole energy inside the device.

For the 15-nm and 20-nm EBL structures, convergence limitations at high bias were also encountered. Nevertheless, when comparing results at the same extraction position, it was observed that the EBL thickness influenced both the hole quasi-Fermi level and the valence-band energy. In particular, the hole current densities near the MQW region for the 15- and 20-nm structures remained at extremely low levels, indicating that hole transport into the MQW region was strongly restricted under the investigated conditions.

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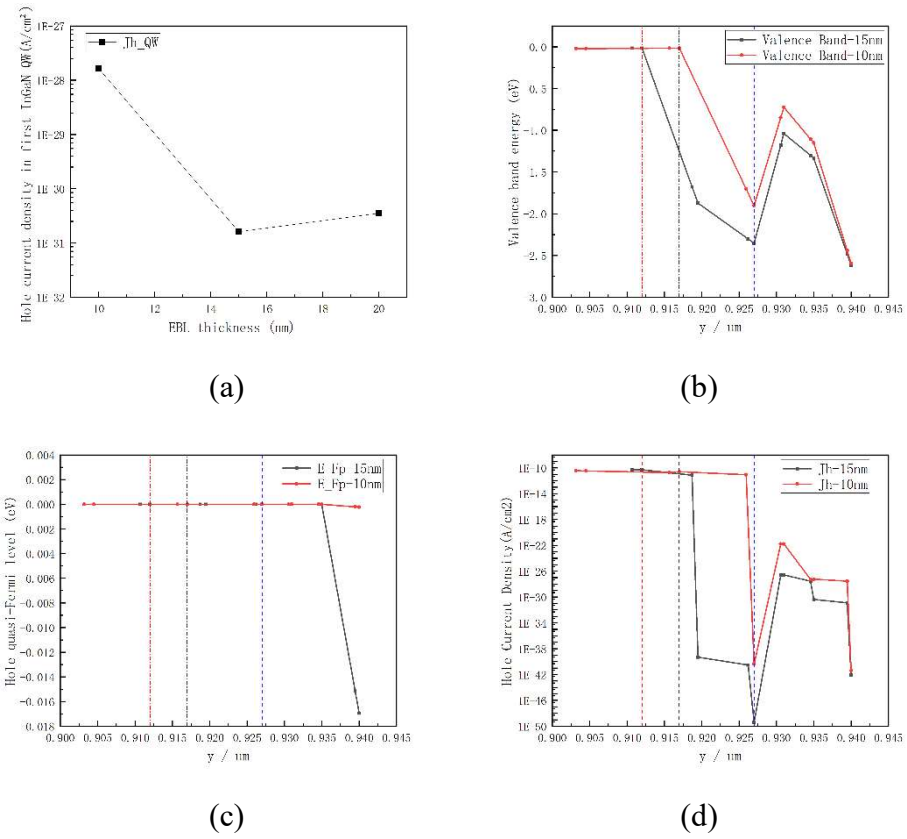

Fig. 2 Effect of EBL thickness on hole transport: (a) hole quasi-Fermi level, (b) valence-band energy, (c) hole current density, and (d) comparison of the hole current density in the MQW region for EBL thicknesses of 10, 15, and 20 nm.

Overall, the simulation results indicate that a thinner EBL shortens the hole transport path and reduces the transport barrier. Therefore, we specifically performed comparative simulations on device structures with 10 nm and 15 nm EBLs. From the simulation results, we extracted and compared the hole quasi-Fermi level, valence band energy, and hole current density, as presented in **Fig. 2** (b), (c) and (d), respectively. Finally, the 10-nm EBL was selected as the EBL thickness for the subsequent optimized structure. It should be noted that this conclusion was obtained mainly from internal hole-transport-related quantities rather than from a complete I–V characteristic.

3.2 Effect of p-GaN Doping Concentration

After determining the EBL thickness, the effect of the p-GaN doping concentration on hole transport was further investigated. Three p-GaN doping concentrations of 5×10^{18}, 1×10^{19} and 2×10^{19}cm^{-3}were considered.

The p-GaN region serves as the main hole injection region, and the Mg acceptor concentration affects both the carrier concentration in p-GaN and the band distribution at the p-GaN/EBL interface. During the simulations, higher p-GaN doping concentrations were found to introduce greater numerical convergence difficulties at higher bias. In particular, a sufficiently reliable high-bias solution could not be obtained for the 2×10^{19}cm^{-3} structure. Therefore, the comparison mainly focused on the structures with 5×10^{18} and 1×10^{19} cm^{-3}.

At the MQW extraction position of y=0.9375 μm, the hole current density was approximately 6.96×10^{-31} A/cm^2 for the 5×10^{18} cm^{-3} structure and 1.61×10^{-31} A/cm^2 for the 1×10^{19}cm^{-3} structure, the results are shown in **Fig. 3** (a). Under the present model and parameter range, increasing the p-GaN doping concentration therefore did not improve hole transport; instead, the lower doping concentration yielded a higher hole current density in the MQW region.

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In addition, the 5×10^{18} cm^{-3} structure exhibited better numerical stability during simulation. Considering both the hole transport result and numerical stability, a p-GaN doping concentration of 5×10^{18} cm^{-3} was selected for the optimized structure.

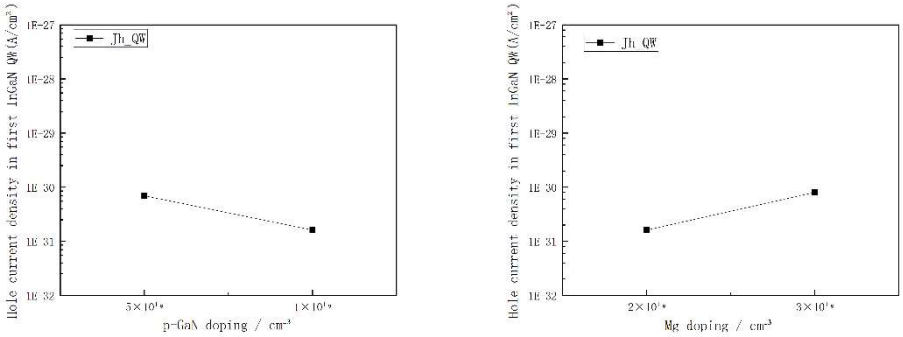
3.3 Effect of EBL Mg Doping Concentration

After determining the EBL thickness and p-GaN doping concentration, the Mg doping concentration in the EBL was further optimized[10]. Three doping conditions of 1×10^{18}、2×10^{18} and $3\times10^{18}cm^{-3}$ were considered.

Mg doping in the EBL can modify the carrier properties of the AlGaN layer and alter the band relationship among the EBL, p-GaN, and MQW regions. Consequently, the Mg doping concentration affects hole transport through the EBL. Among the simulated structures, reliable internal results were obtained for the 2×10^{18} and $3\times10^{18}cm^{-3}$ cases.

At y=0.9375 μm, the hole current density was approximately 1.61×10^{-31} A/cm^2 for the $2\times10^{18}cm^{-3}$ structure and 8.01×10^{-31} A/cm^2 for the $3\times10^{18}cm^{-3}$ structure, the results are shown in **Fig. 3** (b). Meanwhile, the hole quasi-Fermi level shifted from approximately -8.47×10^{-3}eV to -4.22×10^{-3}eV as the EBL Mg doping concentration increased, indicating a change in the internal hole energy distribution.

Therefore, within the investigated range, increasing the EBL Mg doping concentration was found to improve hole transport into the MQW region. Accordingly, $3\times10^{18}cm^{-3}$ was selected as the EBL Mg doping concentration for the optimized structure.



(a) (b)

Fig. 3 Effect of EBL Mg doping concentration on hole transport and the corresponding variation in the hole quasi-Fermi level.

3.4 Comparison of Baseline and Optimized Structures

Based on the above parameter-screening results, the optimized structure was determined as:

a) t_{EBL}=10nm;

b) $N_{p\text{-}GaN}=5\times10^{18}$ cm^{-3};

c) $N_{Mg,EBL}=3\times10^{18}cm^{-3}$.

The optimized structure was then compared with the baseline structure, which employed an EBL thickness of 15 nm, a p-GaN doping concentration of $1\times10^{19}cm^{-3}$,and an EBL Mg doping concentration of 2×10^{18}.

At 0.30 V, reliable internal solutions were obtained for both structures. The hole quasi-Fermi level, valence-band energy, and hole current density in the MQW region were compared to evaluate the combined effect of the optimized parameters on hole transport. The comparison results of the two structures are shown in **Fig. 4** (a), (b), (c) and (d).

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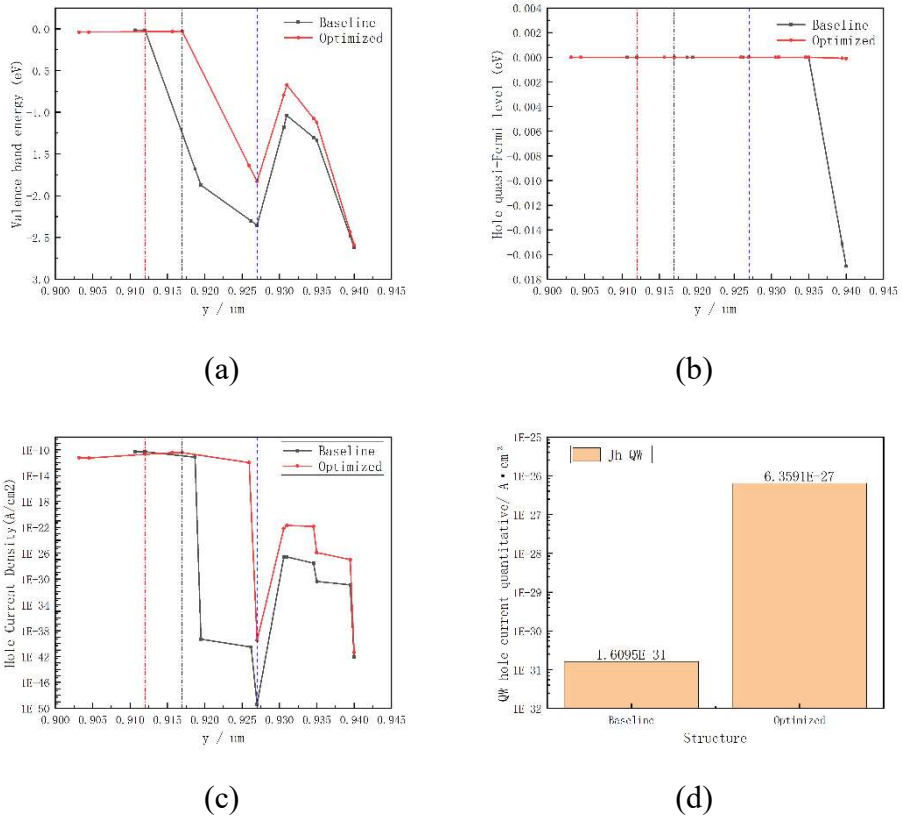

(a) (b)

(c) (d)

Fig. 4 Comparison of (a) the band structure, (b)hole quasi-Fermi level, and (c) hole current density between (d) the baseline and optimized Micro-LED structures at 0.30 V.

Furthermore, the two structures were compared under a common high bias of 1.20 V. The hole current density in the MQW region reached approximately 7.68×10^{-27} A/cm^2 for the optimized structure, compared with 1.91×10^{-31} A/cm^2 for the baseline structure, the comparison results are shown in **Fig. 5**.

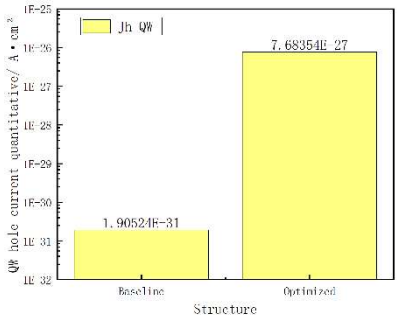

Fig. 5 Comparison of the MQW hole current density between the baseline and optimized structures at 1.20 V.

Therefore, under the present simulation conditions, the optimized structure exhibited a substantially higher hole current density in the MQW region than the baseline structure. Under high bias, the two structures also exhibited different hole quasi-Fermi levels, indicating that their hole energy states were not identical.

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These findings suggest that a thinner EBL, a suitably adjusted p-GaN doping concentration, and a higher Mg doping level in the EBL can alter carrier transport across the p-GaN/EBL/MQW stack. In the present model, such modifications lead to an increased hole current density in the MQW region. The effectiveness of the proposed EBL parameter optimization strategy in improving hole transport in Micro-LEDs was therefore demonstrated.

4. Conclusion

A two-dimensional GaN-based micro-LED structure was simulated in Silvaco TCAD to examine hole transport within the p-GaN/EBL/MQW stack. The influence of EBL thickness, p-GaN doping level, and Mg doping concentration in the EBL was analyzed by comparing the hole quasi-Fermi level, the valence-band energy distribution, and the hole current density. When different EBL thicknesses were compared, the results indicated that this thickness strongly affects hole movement from p-GaN into the MQW region; among the values tested, the 10-nm EBL gave the most favorable hole-transport behavior. For p-GaN doping, the concentration of 5×10^{18} cm^{-3} yielded a higher hole current density and better numerical stability under the present simulation settings, while a higher Mg doping level in the EBL altered the hole energy distribution and increased the MQW hole current density. Based on these results, the final optimized design used a 10-nm EBL, a p-GaN doping concentration of 5×10^{18} cm^{-3}, and an EBL Mg doping concentration of 3×10^{18} cm^{-3}. At the same high bias of 1.20 V, the optimized device showed a markedly larger MQW hole current density of about 7.68×10^{-27} A/cm^2, whereas the baseline structure reached only 1.91×10^{-31} A/cm^2. These findings confirm that adjusting the EBL thickness and p-type doping conditions can enhance hole transport in the simulated GaN micro-LED, offering a numerical guideline for designing the p-type and EBL regions in GaN-based micro-LEDs.

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