Leveraging Machine Learning for Optimization of Internal Quantum Efficiency in Green LED

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***Abstract*— The advancement of green light-emitting diodes (green-LEDs) is essential for full-colour displays and efficient solid-state lighting. However, optimizing the internal quantum efficiency (IQE) of LEDs remains a complex challenge due to the interplay of numerous material and structural factors. This study explores the application of machine learning techniques to optimize the IQE of green-LEDs, using large datasets and advanced algorithms to uncover patterns and suggest optimal configurations.**

Keywords— III-Nitride, Green-gap, Machine Learning

I. Introduction

InGaN-based LEDs play a crucial role across various applications, ranging from efficient general lighting to vibrant full-colour displays. Despite their broad utility, achieving maximum internal quantum efficiency (IQE) remains a formidable challenge due to the numerous interdependent factors influencing performance [1]. These include material composition, crystal quality, defect densities, and device structure, all of which contribute to the complex nature of performance optimization. Machine learning (ML) presents a promising solution to navigate this complexity by offering sophisticated tools for analyzing extensive datasets, modelling intricate relationships, and predicting optimal configurations. ML insights can significantly streamline experimental efforts, minimizing the trial-and-error approach inherent in traditional methods and accelerating the advancement of high-efficiency LEDs.

In this research, we leveraged ML models to address the well-known Green-gap phenomenon. These models were trained on data generated from One-dimensional Schrödinger–Poisson drift-diffusion solver simulations [2], and their accuracy and robustness were evaluated using root mean square error (RMSE). Notably, ML facilitated a systematic exploration of critical parameters in green-LED design, providing valuable insights for future theoretical and experimental investigations.

II. Device Structure

Fig. 1 represents the schematic of a typical InGaN based-LED structure and the various critical parameters. This reference LED includes a 200 nm thick Si-doped (5×10^{18} cm^{-3}) GaN layer, followed by six pairs of multiple quantum wells (MQWs), each consisting of a 3 nm thick $In_{0.24}Ga_{0.76}N$ QW and a 30 nm thick GaN barrier. This is followed by a 50 nm thick p-$Al_{0.3}Ga_{0.7}N$ electron-blocking layer (EBL) and a 150 nm thick Mg-doped (2×10^{19} cm^{-3}) GaN layer.

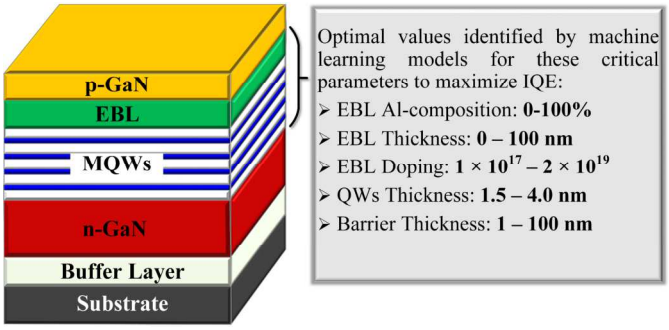


Fig. 1. Reference device structure with a valid defined range of variation for critical parameters.

III. Model Selection

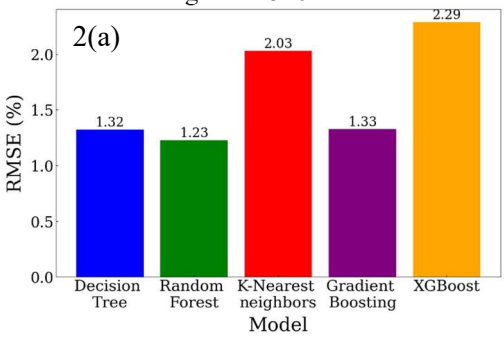
Data for this study were collected from a range of simulation results, encompassing various critical parameters as illustrated in Fig. 1. The dataset was split into training and validation sets, with 20% reserved for validation, followed by hyperparameter tuning using cross-validation to ensure the robustness of the models. As shown in Fig. 2 (a) and (b), the tree-based Random Forest model consistently demonstrated superior performance compared to other models in predicting IQE, achieving the minimum RMSE value, which is defined as

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}\left(IQE_{predicted} - IQE_{Actual}\right)^2}{N}}$$

where, $IQE_{predicted}$ and IQE_{Actual} represent the IQE predicted by the ML model and the simulated IQE, respectively, and N denotes the number of IQE data points in the training dataset.

IV. Results and Discussion

The optimization process starts with a default design of the reference-LED structure, achieving a maximum IQE of 65.2% and an emission wavelength of ~520 nm.



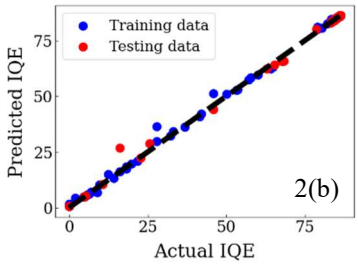


Fig. 2. (a) Represents the comparison of RMSE for different ML models, and (b) IQE predicted values from the Random Forest model with the actual values.

a) Optimum Design of EBL

As depicted in Fig. 3 (a), it is evident that IQE is strongly dependent on the EBL composition. Initially, as the Al-composition increases, the IQE improves due to enhanced electron confinement and a reduction in electron leakage. However, beyond a certain point, further increases in Al-composition result in a sharp decline in IQE, eventually approaching zero when the Al-composition reaches 100% (AlN). This sharp decline is attributed to the excessive increase in the effective potential barrier height for holes at corresponding EBL. When the barrier height becomes too high, holes are unable to reach the active region, thereby preventing them from participating in the radiative recombination process with electrons. This underscores the importance of optimizing EBL composition to balance electron confinement, leakage electron, and hole injection efficiency, ensuring maximum IQE. As shown in Fig. 3 (b), the IQE saturates with respect to thickness after ~15 nm, indicating that beyond this point, further increases in EBL thickness do not impact the IQE value. This suggests that optimizing the EBL thickness to around 15 nm is sufficient for maximizing IQE, as additional thickness does not contribute to performance improvements.

The doping concentration of the EBL also plays a crucial role in improving its effectiveness. It has been observed, through ML analysis, that varying the p-type doping concentration 1×10^{17} cm^{-3} to 2×10^{19} cm^{-3} reveals an optimal p-type doping level that matches the doping level of the p-GaN layer.

b) Optimum Design for Active Region

QW thickness directly influences the optical and electrical properties of the LED, including its emission wavelength and carrier confinement. Conventional c-plane LEDs typically utilize QWs thickness ranging from 1.5 to 4.0 nm. Optimal QW thickness is essential for achieving efficient electron-hole recombination, thereby maximizing the IQE for a target

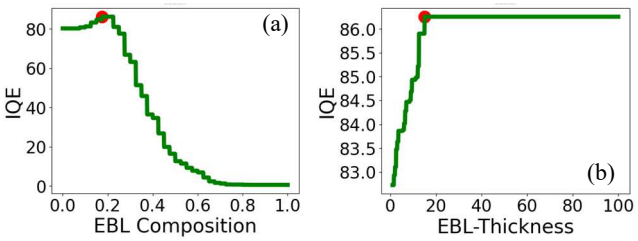


Fig. 3. (a) Predicted IQE curve for EBL (a) composition, and (b) thickness. The red dot represents the optimal value.

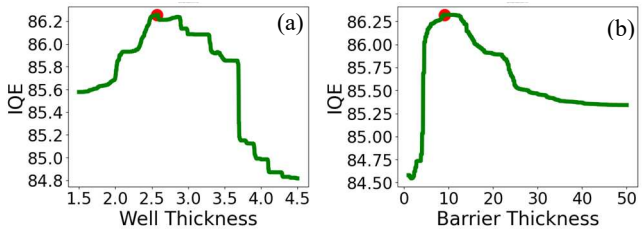


Fig. 4. (a) Predicted IQE curve for the active region: (a) QW thickness, and (b) barrier thickness. The red dot represents the optimal value.

wavelength. Thinner QWs result in shorter emission wavelengths, while thicker QWs induce a stronger quantum-confined Stark effect, leading to longer wavelengths for a given In-content. For a target emission wavelength of 520 nm, ML optimization suggests an ideal QW thickness of 2.566 nm, as shown in Fig. 4 (a). Moreover, barrier thickness plays a crucial role in carrier confinement within the MQW by providing an adequate barrier to electrons, and it also impacts the current-voltage characteristics of the LED. ML optimization indicates that an ideal barrier thickness of ~9 nm is optimal for achieving the target emission wavelength with maximum IQE, as demonstrated in Fig. 4 (b).

Lastly, precise adjustments of critical parameters were made as suggested by the ML model. We simulated an optimized structure with these parameters, resulting in a significant improvement in IQE and reduced efficiency droop compared to the default design of the reference LED, as illustrated in Fig. 5.

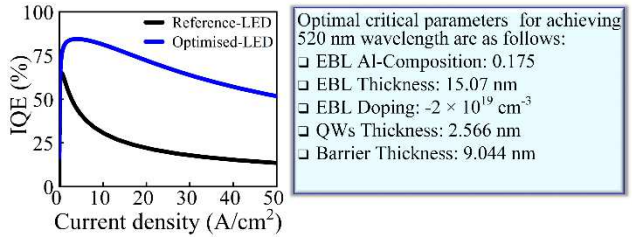


Fig. 5. Calculated IQE of ML-based Optimized-LED Compared to the Reference-LED structure with mentioned optimal Critical parameters in the box.

V. Conclusion

This paper demonstrates how integrating ML accelerates the quest for high-efficiency LEDs, surpassing traditional trial-and-error methods. Traditional approaches often struggle due to the nonlinear and high-dimensional nature of various critical parameters in optoelectronic device design. By leveraging ML, precise adjustments of critical parameters within their defined ranges significantly enhance IQE by 32% compared to the Reference LED.

References

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