Development of a CAE-Based OLED Modeling Environment for Electrical and Optical Simulation

Han Wool Park*, Yoon Ji Choi*, Han-Seung Yang*, Jong Seuk Kang*, Hanjin Park*, Sun-Kyung Cha*, Dong Shin Choi*, Yosub Lee*, Heui-Dong Lee*, Sung Ki Kim*, Han Hee Kim*, Jeongguk Min*, Seok-Woo Lee*, Joon-Young Yang*, Sooyoung Yoon*

***LG Display Co., Ltd., Seoul, Republic of Korea**

Abstract

This study presents a CAE-based OLED modeling environment to replace traditional evaluation methods. A physics-based model was developed to simulate charge conduction mechanisms, with key material properties extracted. The model's accuracy, validated through electrical/optical analyses and DOE studies, demonstrated significantly improved predictive precision and efficiency, reducing design iteration time and enhancing performance optimization. This robust tool offers a scalable and cost-effective solution for OLED development.

Author Keywords

OLEDs; Computer aided engineering; Modeling; Simulation; Physics-based model; Design of experiments;

1. Introduction

Organic light-emitting diode (OLED) devices are complex electronic systems composed of multiple functional layers, including the emissive layer, electron transport layer, hole transport layer, and various charge injection layers. Each of these layers has unique physical properties, such as charge mobility, energy levels, and refractive indices, as well as varying thicknesses and material concentrations [1,2]. These parameters collectively play a critical role in determining the overall device performance, including luminance, efficiency, and lifetime. However, optimizing such a multilayer structure presents significant challenges due to the complex interactions between layers. Small changes in one layer can lead to substantial variations in device behavior, necessitating numerous iterative experiments to identify the optimal configuration. This iterative process is not only time-consuming but also resource-intensive, resulting in increased development costs and extended time-to-market [3].

To overcome these challenges, computer-aided engineering (CAE) has gained prominence as a powerful tool in the OLED development process. CAE allows for virtual prototyping and testing, significantly reducing the reliance on physical experiments. By utilizing CAE, researchers and engineers can rapidly explore a wide range of design parameters, such as layer thickness, material composition, and device architecture. This approach enables efficient design optimization by identifying promising configurations early in the development cycle, thereby reducing both time and costs. Furthermore, simulation environments based on CAE facilitate a deeper understanding of the underlying physics by predicting electrical and optical characteristics, including current density, luminance, and emission spectra, under various operating conditions. These predictive capabilities provide invaluable insights, helping to streamline the development process and minimize trial-and-error experimentation [4,5].

However, the effectiveness of CAE in OLED development depends heavily on the accuracy of the underlying models. OLED devices operate based on complex physical mechanisms, including charge injection, transport, recombination, and exciton formation. Accurately capturing these phenomena requires a detailed understanding of the material properties, such as charge mobility, energy band alignment, and exciton lifetimes, as well as precise modeling of the physical processes governing charge transport and recombination. Without these considerations, simulation results may deviate significantly from actual device behavior, limiting the utility of CAE in predicting performance [6].

Recognizing these challenges, our study aims to develop a robust physics-based model that incorporates the essential material properties required for accurately simulating charge conduction mechanisms in OLEDs. This model forms the basis of a CAE-based OLED modeling environment designed to support device analysis and optimization. By combining advanced material characterization techniques with molecular dynamics (MD) and density functional theory (DFT) simulation, we have developed a modeling system that demonstrates promising accuracy and reliability. The validity of this system was assessed through detailed comparisons with experimental data, including electrical and optical measurements, as well as design of experiments (DOE) studies to explore the effects of layer thickness and material concentration on device performance.

2. OLED modeling and simulation process

Figure 1 illustrates a schematic of the OLED modeling and simulation process. The OLED modeling and simulation process begins with collecting experimental data, such as current density-voltage (J-V) characteristics, luminance efficiency, and emission spectra. These data provide essential insights into material properties and device behavior, serving as a foundation for the simulation environment.

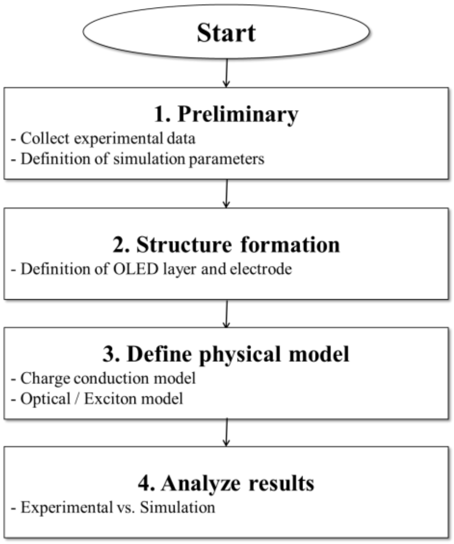

Figure 1. Flowchart of the OLED modeling and simulation process.

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Based on this data, key simulation parameters, including charge mobility, energy levels, and layer thicknesses, are defined to ensure the simulation accurately reflects OLED performance. The virtual OLED structure is then constructed, modeling each functional layer (emissive, electron transport, and hole transport) and their interactions to replicate real device dynamics. Next, physical models are developed to describe mechanisms such as charge injection, transport, recombination, and exciton formation. These models are calibrated using experimental data to ensure accuracy. Finally, simulation outputs are analyzed and validated against experimental results by comparing metrics like J-V characteristics and EQE. Sensitivity analysis and DOE studies further explore the impact of design variations, optimizing device performance. This iterative process enhances simulation precision, reduces reliance on physical prototypes, and accelerates OLED development.

3. Results and discussion

3.1. Extraction methods for material properties

To develop a highly accurate OLED modeling environment, we established methods for extracting the key parameters that define the modeling environment. Given the amorphous nature of organic materials used in OLEDs, we specifically developed techniques to extract the physical properties of thin-film materials, accurately reflecting the characteristics of actual device structures. Energy levels, which are critical for determining charge injection and transport properties, were accurately measured through detailed experimental techniques [7]. Meanwhile, the number of electrons (N_e) and holes (N_h), along with charge mobility, were calculated using advanced computational methods, including MD/DFT simulations [8]. These simulations provide atomic-level insights into charge transport mechanisms, accounting for the influence of molecular packing and disorder. Additionally, excitonic and optical properties were derived from experimental methods [7]. By integrating experimental and computational techniques, we created a comprehensive dataset. This approach ensures our OLED modeling environment provides accurate simulations, aligning closely with experimental results and optimizing device performance under various conditions. (Table 1)

Table 1. Parameter extraction methods used in OLED modeling.

Parameters	Extraction methods
Energy level	Experiment
N_e	MD/DFT
N_h	MD/DFT
Mobility	MD/DFT
Exciton	Experiment
Optical	Experiment

3.2. Physics-based OLED model design

To establish a highly accurate OLED modeling environment, we developed not only default physics models but also supplementary models to analyze charge behavior (Figure 2). Among these, the gaussian density of states (G-DOS) model was incorporated to improve simulation accuracy. The G-DOS model, applied to all OLED layers, offers a detailed representation of charge distribution within the device (Figure 3). Key Gaussian distribution parameters, including energy level centers and standard deviations, were derived from MD/DFT [9]. These parameters capture the inherent disorder in organic materials and are crucial for accurately modeling the spatial and energetic distribution of charge carriers.

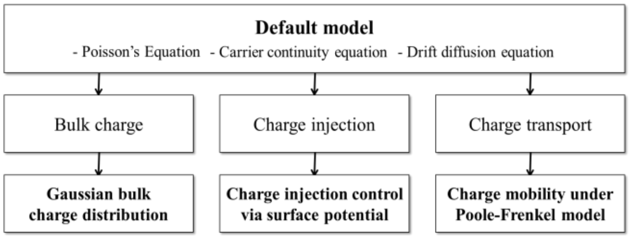

Figure 2. Physical models utilized in OLED modeling.

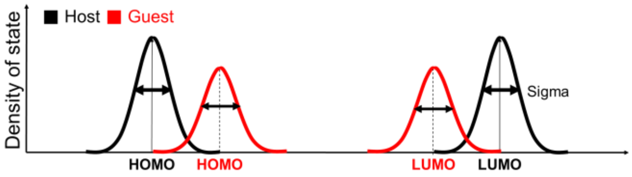

Figure 3. Scheme of gaussian density of states.

Additionally, a surface potential (SP) model was implemented to control band bending at heterojunction interfaces. This model plays a critical role in simulating charge injection dynamics, particularly at the interfaces between different OLED layers [10]. For example, when a positive surface potential (SP) is introduced in the hole transport layer (HTL) (Figure 4a), it induces a redistribution of charges at the heterojunction interface, leading to a stronger repulsive force for holes. This causes the HTL's highest occupied molecular orbital (HOMO) level to shift to a lower energy state relative to the fermi level, effectively increasing the energy gap between them. As a result, the hole injection barrier rises, reducing hole injection efficiency and impeding charge transport across the interface. Conversely, when a negative SP is applied to the HTL (Figure 4b), it reduces the repulsive force for holes, allowing the HOMO level to shift closer to the Fermi level. This decreases the hole injection barrier, enhancing hole injection efficiency and improving charge transport. As shown in Figure 5, we developed a surface potential model and verified through simulations that it operates consistently with the underlying mechanism. This demonstrates that the designed environment effectively controls band bending behavior.

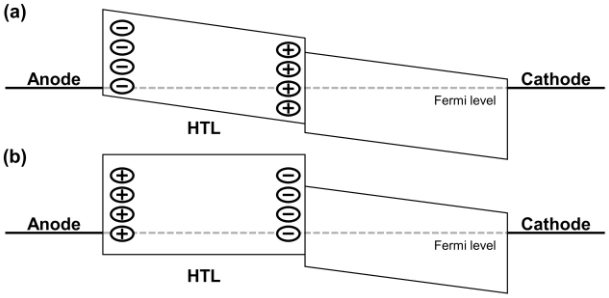

Figure 4. Energy diagram illustrating the effects of (a) positive, and (b) negative surface potentials in the HTL.

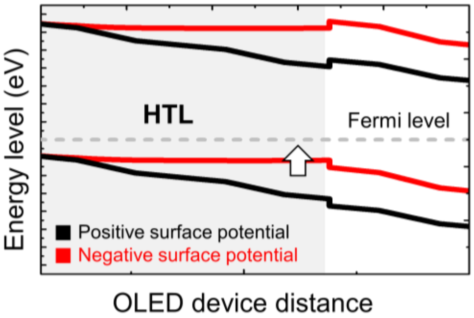

Figure 5. Energy diagram illustrating band bending under the simulated surface potential of HTL.

To further enhance the modeling environment, we incorporated the Poole-Frenkel (PF) mobility model to account for field-dependent charge mobility [11]. Mobility plays a critical role in determining charge transport efficiency, and accurately modeling its behavior under different operating conditions is essential for simulating OLED performance. The PF model accounts for the influence of the electric field on charge carrier mobility, which is crucial for capturing the dynamic behavior of OLEDs, particularly under varying voltage conditions. This allows for a more realistic simulation of charge injection and transport, as mobility changes significantly depending on the electric field strength. As shown in Figure 6, the constant mobility model assumes that mobility remains fixed, regardless of voltage fluctuations. While this approach simplifies the simulation, it fails to represent the actual behavior of OLEDs, especially in high-field regions where mobility tends to increase. This oversimplification can lead to inaccuracies in predicting device performance, particularly when analyzing regions with varying operational voltages. In contrast, the PF mobility model dynamically adjusts mobility in response to voltage changes, reflecting the inherent field-dependent behavior of charge carriers. This enables the model to provide a more precise representation of OLED characteristics across different operating regions, including low- and high-field conditions. As a result, the PF model allows for a more accurate alignment between simulated and experimental data, improving the reliability of the modeling environment.

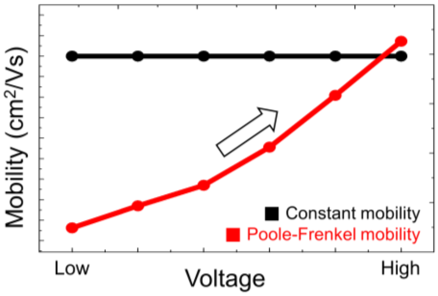

Figure 6. Simulated electric field dependence of effective charge carrier mobility models.

By incorporating the G-DOS, SP, and PF models, we developed a robust system for analyzing charge behaviors in OLEDs. These models improve the accuracy of simulating charge conduction mechanisms. This approach enhances simulation consistency, aligning more closely with experimental data and offering insights for optimizing OLED performance under various conditions.

3.3. Analysis of OLED electrical and optical modeling results

Using the extracted physical properties of organic materials and the developed physics-based models for OLED operation, we designed a comprehensive electrical and optical modeling environment for OLEDs. To evaluate the accuracy and reliability of this environment, we analyzed the electrical characteristics of OLED devices. As shown in the J-V results (Figure 7a), the simulation outputs from our modeling environment demonstrate excellent agreement with experimental data, confirming the high accuracy of the simulations. Additionally, the capacitance-voltage (C-V) results (Figure 7b) also exhibit strong consistency between simulation and experimental outcomes.

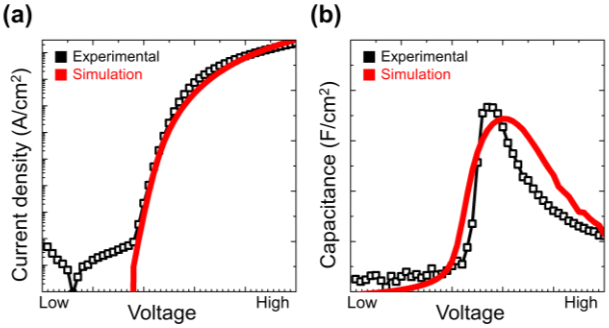

Figure 7. (a) Current density-voltage characteristics, (b) Capacitance-voltage characteristics of the OLED device. Experimental results (black) and simulated results (red).

We also conducted a detailed analysis of the optical characteristics of the OLED devices to further validate the accuracy of our modeling environment. We examined photoluminescence (PL) and luminance-voltage (L-V) behaviors. The PL spectrum (Figure 8a) results provided insights into the excitonic properties and light emission efficiency, while the L-V (Figure 8b) analysis highlighted the device's luminance performance under varying voltage conditions. In both cases, the simulation outputs showed excellent agreement with experimental data, confirming that the modeling environment accurately captures the optical behavior of OLEDs. This high level of consistency underscores the reliability of our approach in simulating not only electrical but also optical properties across different operating conditions.

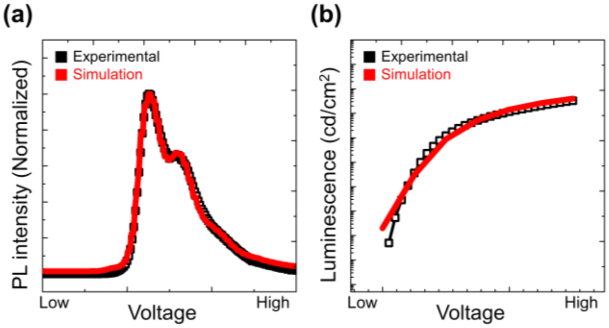

Figure 8. (a) PL spectrum characteristics, (b) Luminescence-voltage characteristics of the OLED device. Experimental results (black) and simulated results (red).

Evaluating the accuracy of the modeling environment is critical when considering its potential to replace experimental methods, and DOE plays a key role in this process. To assess the reliability of our OLED modeling environment, we conducted DOE analyses focusing on layer thickness and material concentration across different operating regions, including low-field and high-field conditions. This approach enabled a thorough evaluation of the modeling environment's accuracy in predicting OLED performance under varying design and operating parameters. We conducted a DOE analysis on the thickness of the electron blocking layer (EBL) across different operating regions to evaluate the accuracy of our OLED modeling environment. The results (Figure 9) demonstrated excellent agreement between the simulation and experimental data, confirming the model’s capability to accurately predict OLED performance under various design and operating conditions.

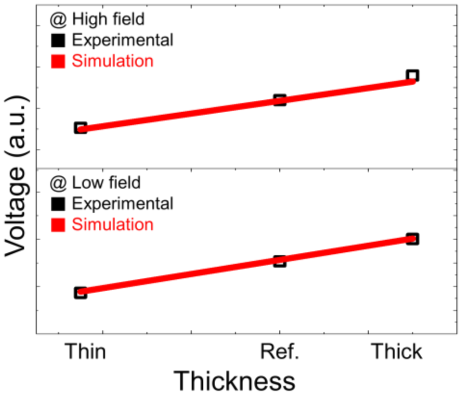

Figure 9. OLED voltage under low field (bottom) and high field (top) operating conditions with varying EBL thickness.

We also conducted a DOE analysis on the doping concentration of the hole injection layer (HIL) across different operating regions. The simulation results (Figure 10) showed strong agreement with experimental data, further validating the modeling environment's ability to accurately capture the impact of HIL doping concentration on device performance. This demonstrates that our environment can reliably predict OLED behavior not only for structural variations but also for material property adjustments, ensuring high accuracy across various operating conditions.

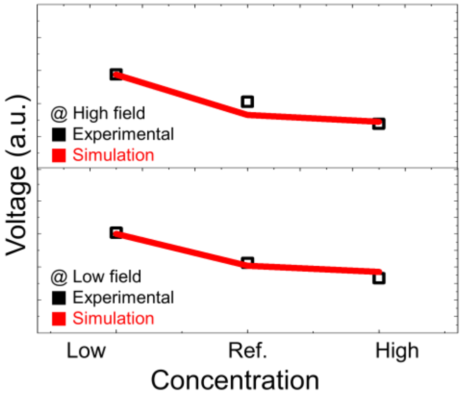

Figure 10. OLED voltage under low field (bottom) and high field (top) operating conditions with varying HIL doping concentration.

4. Conclusion

This study presents the development of a highly accurate and reliable OLED modeling environment, aimed at enhancing both performance prediction and design optimization. To achieve this, we implemented advanced techniques for extracting material properties and constructed physics-based models tailored to OLED operation. Validation through electrical and optical analyses demonstrated strong agreement between simulation and experimental data, confirming the precision of the modeling environment. We further evaluated the system using DOE analyses, examining variations in layer thickness and material concentration across different operating regions. These results underscored the environment’s ability to accurately predict device behavior under various design and operational conditions. Overall, the proposed modeling environment offers a robust solution for simulating OLED performance, reducing reliance on physical experimentation. While further refinement is ongoing, this study aims to establish a modeling environment that can significantly enhance OLED design optimization. This approach not only accelerates the development process but also provides valuable insights into device optimization, contributing to more efficient and cost-effective OLED design.

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