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SIMULATION AND ANALYSIS OF ELECTRO-OPTICAL CHARACTERISTICS OF ORGANIC COMPOUNDS IN ORGANIC LIGHT-EMITTING DIODES (OLEDS)

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ABSTRACT

Organic light emitters (OLEDs) work according to the principles of electroluminescence. These OLEDs are commercially available and can be used in smartphone and television displays due to their low power consumption, flexibility and higher brightness than inorganic de-vices. The copolymer based on 3,4-ethylene dioxythiophene (EDOT) and poly(N-vinylcarbazole) (PVK) was synthesized using previously published procedures. The copolymer was synthesized by an oxidative copolymerization reaction, while the DFT/B3LYP/6-31G(d,p) density function theory method was used to perform quantum calculations. This paper presents the simulation results by SILVACO-TCAD simulation software of the PVK-PEDOT organic matrix with calcium as cathode and ITO as anode. The simulation is based on the distribution of the Langevin recombination model including the proposed structure, and the electrical and optical characteristics, such as current versus voltage, luminescence power, and current versus electric field for different thicknesses, and charge carrier densities of the emitting layer, as well as the I-V characteristics for different temperature values. The model presented here will be useful in the future for optimization of better electrical parameters.

Keywords: Organic Compounds, SILVACO, PVK-PEDOT, OLED, Electro-Optical Characteristics

1. INTRODUCTION

Currently, molecular materials based on π-conjugated systems are in full development. These systems were discovered in the 1970s by A. Hegger, Mc Diarmid and H. Shirakawa Heeger et al. (2002) during their research on doping polyacetylene. Since then, many polymers and materials based on conjugated compounds have been thoroughly investigated by several research teams Al-Azzawi et al. (2023). Due to their physicochemical and optoelectronic properties, these systems are being considered for various applications in the field of organic electronics. Although the electroluminescence of organic materials was studied as

early as the 1960s thanks to the work of Pope and Helfrich Helfrich and Schneider (1965), it was not until the 1980s that this phenomenon began to interest industrialists due to the rise of organic electronics Partridge (1983).

Materials based on π-conjugated organic compounds have attracted significant attention in the fields of chemistry, physics and materials science Zeng et al. (2018). This is due to their attractive characteristics, which include high charge mobility, high throughput, lightness, flexibility, photochemical and thermal stability Güney et al. (2019), and the possibility of rapid and cost-effective roll-to-roll fabrication Raftani et al. (2021).

Indeed, this new discipline introduces organic materials instead of classical inorganic semiconductors to realize organic light-emitting diodes OLEDs, field effect transistors, photonic crystals, modulators, organic solar cells (OSCs), optoelectronic components, lasers El karkri et al. (2022).

The first OLED was created by Tang and Van Slyke in 1987 Luo et al. (2022). Since this invention, OLEDs have continued to be studied and used for many industrial applications. In 1987, Tang and Van Slyke created the first OLED, since then OLEDs have been widely studied and used in many industrial applications. A number of OLED-based applications are already being implemented, including the production of thin and flexible TV displays, GPS navigation, portable media players, radios, smartphones and clothing. A significant increase in production volume is expected in the coming years as OLED lighting applications and printed OLEDs enter the market Bizzarri et al. (2018).

OLEDs are already used in models from Motorola, Samsung, LG, Nokia and some models from Sony Ericsson Udhiarto et al. (2015).

OLEDs offer several advantages over competing technologies such as LCDs and LEDs. First, OLEDs are relatively brighter, more flexible and less expensive, while offering faster response than comparable devices. In addition, OLEDs emit light directly at the pixel level, eliminating the need for a backlight, unlike LCDs. This improves image quality in terms of color, contrast and viewing angle, but more importantly, it allows for more compact and lighter displays. This advantage is reinforced by the fact that OLED technology is a thin film technology. The first OLED display commercialized by LG in 2013 was no more than 4 mm thick for 3.5 kg.The compact and robust aspect of OLEDs as well as the possibility of manufacturing the screen on all types of supports (flexible, conformable, transparent) make them particularly suitable for use in nomadic systems Singh et al. (2012).

As OLEDs are a recent technology, their operation is not yet fully understood. To better understand their behavior, it is necessary to perform many experimental and modeling studies. However, these researches are costly and time consuming. To circumvent these constraints, computer-aided design (CAD) tools can be used to model and simulate the processes of OLEDs. There are several organic models that are used to simulate the behavior of OLEDs, such as Poole-Frenkel mobility, jump models, and the Langevin recombination model Raj et al. (2019).

The present study concerns the simulation of an OLED through an ITO/PVK-PEDOT/Ca device structure. The details of the simulation process, the selection of physical models and the obtaining of the Langevin recombination distribution are explained in the first part of this study. The second part provides information on the structure of the device, the electronic properties of the layers and the operating principles obtained by DFT Taherinia and Fattahi (2022). Kharchich and Khamlichi, (2023). The third part presents simulation results and electrical and optical

characteristics achieved by SILVACO-ALTAS Bakour et al. (2022), and the last part draws conclusions and highlights future perspectives for the use of OLEDs.

2. MATERIALS AND METHODS

With TCAD (Computer Aided Design for Technology) simulators, it is possible to model both the physical and electrical aspects of electronic components, as well as their optical characteristics. This approach reduces development costs and optimizes the time required to design components. The objective of this simulation is to optimize the performance of the device. The software environment provided by SILVACO (Silicon Valley Corporation) is designed for the design and performance prediction of semiconductor devices. Silvaco TCAD is a valuable resource for designing semiconductor devices prior to the manufacturing process, and has proven beneficial in various research projects. The software incorporates state-of-the-art physical models, numerical methods, algorithms, improved meshing techniques, and linear solution optimization, making it a very effective tool for semiconductor design, resulting in simulation results that closely match real-world results. The main advantage of this simulator is the possibility to visualize complex physical phenomena that would normally be difficult to observe Kharchich and Khamlichi, (2023).

3. ELECTRONIC PROPERTIES

In this study, we aim to investigate and simulate the electronic properties of PVK-PEDOT, focusing on the electronic properties of organic light-emitting diodes. The synthesis of PVK-PEDOT is illustrated in Figure 1 El Malki et al. (2010). The electronic properties of an oligomer are mainly influenced by the energy levels of the highest occupied molecular orbital (HOMO) and the lowest occupied one (LUMO) Semire et al. (2020). To evaluate the electron and hole transport capacity, an analysis of the HOMO and LUMO of the oligomer is performed. The HOMO represents the electron donating capacity of the oligomer, while the LUMO represents its electron accepting capacity. In general, it is expected that a molecule with a higher HOMO density will have a higher electron donating capacity, and a molecule with a higher LUMO density will have a higher electron accepting capacity Liang et al. (2021).

The band gap (Egap) of the examined molecules was determined by subtracting the HOMO and LUMO energy levels (ΔEHOMO-LUMO) using the B3LYP/6-31 G(d,p) method Azaid et al. (2021). Figure 2 shows the HOMO and LUMO energies and the calculated energy differences, comparing the results of the theoretical methods with the experimental data. The results obtained by the DFT method were the most reliable, giving a band gap of 2.71 eV after correction, which is in agreement with the band gap extrapolated from the experimental absorption spectra (2.45 eV) El Malki et al. (2010). In general, it is accepted that the theoretical band gaps calculated for isolated chains are about 0.2 eV higher than the condensed phase values Raftani et al. (2020), and our results are consistent with this expectation. Thus, the calculated band gaps indicate that the PVK-PEDOT copolymer exhibits promising electronic properties, The theoretical results are in agreement with the experimental data.with theoretical results in agreement with the experimental data.

Equation 1 EL Mhamedi et al. (2022) is used to calculate the electron affinity EA, which reflects the ability of a material to accept an electron.

$$EA = E(M) - E(M^{-}) \quad (1)$$

The energy of the neutral molecule (E(M)) and the energy of the neutral molecule and the anion (E(M)) were calculated using the B3LYP/6-31G(d,p) level. The HOMO, LUMO, band gap (Egap) and electron affinity (EA) values of the PVK-PEDOT copolymer are shown in Table 1.

Figure 1

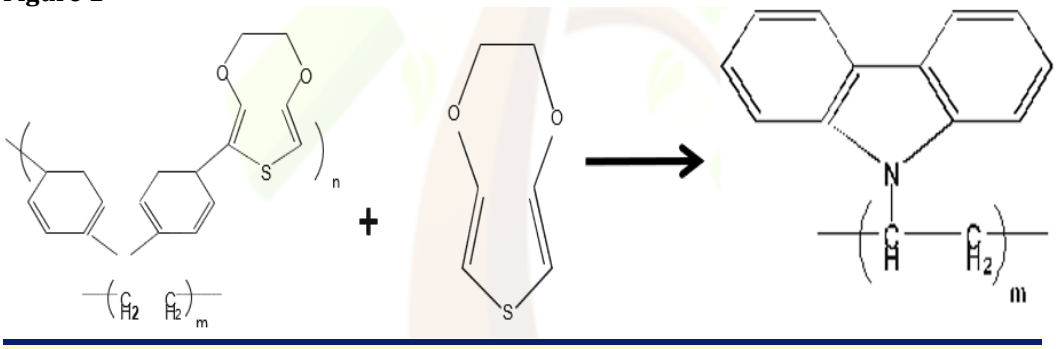

Figure 1 PVK–PEDOT Synthesis [20]

Figure 2

Figure 2 The Egap Energies Calculated (a) and Experimental (b) of PVK-PEDOT El Malki et al. (2010)

The copolymer absorbs light in the visible (450-800 nm) and ultraviolet (200-450 nm) regions, with a broad band centered at about 620 nm observed in the visible region. This band is attributed to a π - π * transition resulting from the presence of PEDOT moieties in the copolymer and the increase in conjugation length by the π spacer component of the molecule Nitschke et al. (2021). Based on these results, the PVK-PEDOT copolymer is considered a promising material for electronic applications; this applies particularly to the creation of organic light-emitting diodes.

Table 1

Table 1 The EHOMO, ELUMO, EGAP and EA Energies of the PVK-PEDOT from the DFT Method El Malki et al (2010)

Parameters	HOMO	LUMO	Egap	EA
Energies Values(eV)	-6.59	-3.68	2.91	2.8

4. PHYSICAL MODEL

OLEDs use different models to describe charge transport. The Poole-Frenkel mobility model and the Langevin bimolecular recombination model are used to explain the polymer transport and the recombination mechanism, respectively. In addition, the singlet exciton model is used to calculate the radiative luminescence rate resulting from Langevin recombination. Each of these models is described both

physically and mathematically. The following equations describe the Poole-Frenkel mobility model Gill (1972).

$$\mu_n(E) = \mu_{n0}\exp\left(\frac{-DELTAEN.PFMOB}{\text{KTneff}} + \left(\frac{\text{BETAN.PFMOB}}{\text{KTneff}} - GAMMA, PFMOB\right)\sqrt{|E|}\right) \quad (2)$$

$$\mu_p(E) = \mu_{\rho 0}\exp\left(\frac{-DELTAEP.PFMOB}{\text{KTneff}} + \left(\frac{\text{BETAP.PFMOP}}{\text{KTneff}} - GAMMP.PFMOB\right)\sqrt{|E|}\right) \quad (3)$$

Where μnPF(E) and μpPF(E) are the Poole-Frenkel mobilities for electrons and holes respectively, μn0 and μp0 are the zero field mobilities for electrons and holes respectively, and E is the electric field. DELTAE N.PF MOB and DELTAEP.PFMOB are the activation energy at zero electric field for electrons and holes respectively. BETAN.PFMOB is the electron Poole-Frenkel factor, and BETAP.PFMOB is the hole Poole-Frenkel factor.

Tneff and Tpeff are the effective temperature for electrons and holes respectively. Due to the strong dependence on the electric field, the Poole-Frenkel mobility model can cause convergence problems. To increase the stability of the Poole-Frenkel mobility model, the following equations are used.

$$\mu_n(E) = \frac{1}{\frac{1}{\mu_n(E)} + \frac{1}{\mu_{nlim}(E)}} \quad (4)$$

$$\mu_p(E) = \frac{1}{\frac{1}{\mu_p(E)} + \frac{1}{\mu_{plim}(E)}} \quad (5)$$

In OLEDs, electron and hole mobilities are represented by μn(E) and μp(E), while their limiting mobilities are represented by μnlim(E) and μplim(E), respectively, calculated from the thermal velocities. The luminescence rate in the OLED is deduced from the distribution of singlet excitons. In Atlas software, the singlet exciton continuity equations are solved simultaneously with the electron and hole drift diffusion equations Ruhstaller et al. (2001). The bimolecular recombination rate is described by the Langevin recombination rate, which is expressed by the following analytical expression.

$$R_L n, p = r_L(x, y, t)(np - ni^2) \quad (6)$$

The intrinsic carrier concentration is represented by ni, and the Langevin recombination rate coefficient is represented by rL (x, y, t). The latter is defined by the following expression Blom et al. (1997).

$$\boldsymbol{R_L(x, y, t)} = \boldsymbol{A}\ \text{LANGEVIN}\ \frac{q[\mu_n(E) + \mu_p(E)]}{\epsilon_r \epsilon_o} \quad (7)$$

The prefactor of the Langevin bimolecular recombination model is denoted A. Langevin and depends on the relative permittivity εr and the absolute permittivity ε0. Its default value is 1.

5. PRESENTATION OF THE SIMULATED STRUCTURE

Organic light-emitting diodes are based on charge carrier injection (the physical phe-nomenon generated by applying an electric field to the organic material is called injection electroluminescence). The object of this study is a simulated organic LED, composed of a PVK-PEDOT layer and a film of organic electroluminescent material sandwiched between two electrodes. Figure 3 shows the electrical circuit diagram, while Figure 4 shows the structural diagram of the OLED. ITO (Indium Tin Oxide) material, composed of indium and tin oxide, is transparent and used as an anode on a glass substrate. It behaves like an n-type semiconductor, with a wide band gap of 3.5 to 4.3 eV.resulting in high transmission rate (>85%) in the visible and infrared spectrum. Its superior properties, such as its anti-reflective coating, electromagnetic field shielding, thermal insulation, and low resistivity, make it an ideal choice for transparent electrode applications Alam et al. (2000). The calcium (Ca) cathode is produced by repeated evaporation of calcium layers. The low work function of 2.9 eV improves the efficiency of electron injection into the organic layers, which facilitates the creation of organic light-emitting diodes. To realize this electron injection into the conduction band via the cathode, the diodes use a sandwich structure. In parallel, holes are injected into the valence band via the ITO anode. When an electric field is applied, the charge carriers move and combine to form excitons. These then disappear by radiation emission, which is the origin of the principle of electroluminescence Janghouri and Mohajerani (2019).

Figure 3

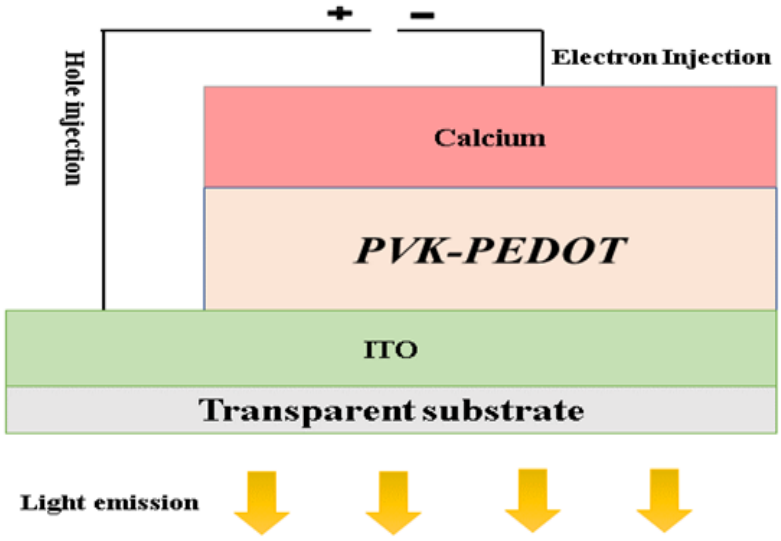

Figure 3 OLED Electrical Circuitry

Figure 4

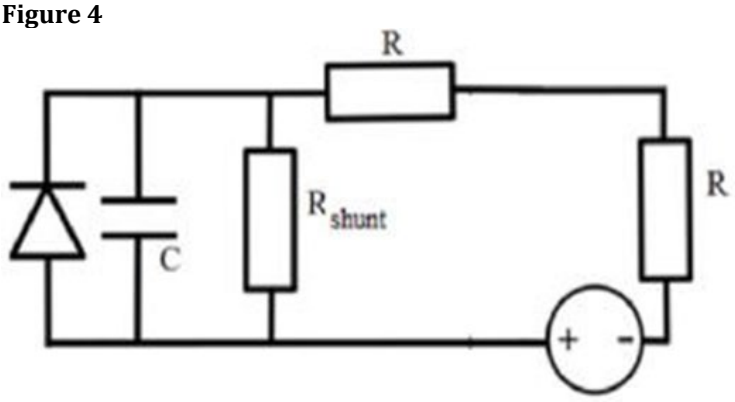

Figure 4 Structure of OLED

6. RESULTS AND DISCUSSION

6.1. STRUCTURE OF THE SIMULATED LED

The simulation of the organic light emitting diode (OLED) structure was performed using the ATLAS simulator, which is capable of providing a comprehensive analysis of organic devices Lysenko et al. (2016). The OLED structure was defined using Atlas syntax, which allows for the definition of vertical and horizontal lines and their spacing. Accurate and efficient numerical modeling depends on a well-defined mesh, which emphasizes its importance. Material parameters such as permittivity, band gap, electron affinity, effective density of states, hole and electron mobility, as well as electrode location and doping level in each region were specified for accurate simulation. The electrical and optical characteristics of the OLED were then obtained by applying these parameters. The parameters used for the simulation of PVK-PEDOT-based OLEDs are listed in Table 1. This study presents a simulation of an organic LED (OLED) using a PVK-PEDOT layer. The device configuration consists of an indium tin oxide (ITO) electrode, the PVK-PEDOT layer, and a calcium (Ca) presented in Figure 5. The results show that the Langevin recombination rate across the active layer surface is high. Specifically, a significant increase in the recombination rate is found on the cathode side, while a slight decrease is observed as the thickness of the PVK-PEDOT layer increases. These results suggest that the simulated OLED structure exhibits desirable electrical characteristics.

Table 2

Table 2 The different parameters used for the simulation of PVK-PEDOT for OLEDs

Parameters	Value
Thickness (nm)	50
Band gap (eV)	2.45
Electron affinity (eV)	2.8
Relative Permittivity	3
Hole mobility (cm2 /vs)	10^{-2}
Electron mobility (cm2 /vs)	10^{-4}
Effective density of states in the conduction band NC300 (cm-3)	2.10^{21}
Effective density of states in the valance band (Nv)ND300 (cm-3)	2.10^{21}

Figure 5

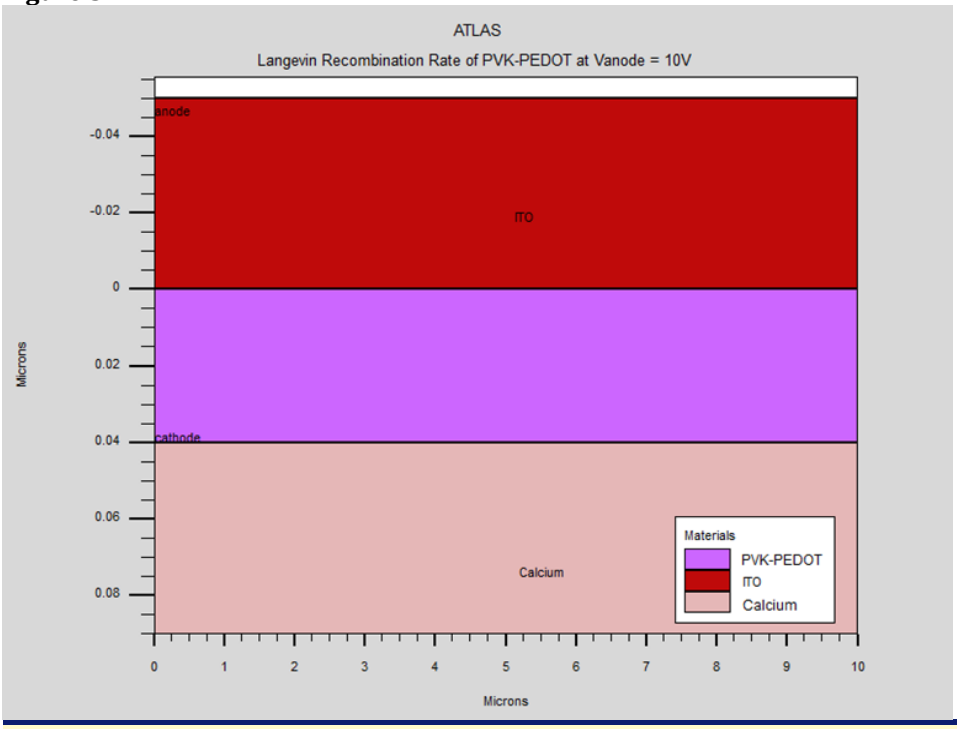

Figure 5 Simulating OLED Structure using Silvaco Atlas

Figure 6

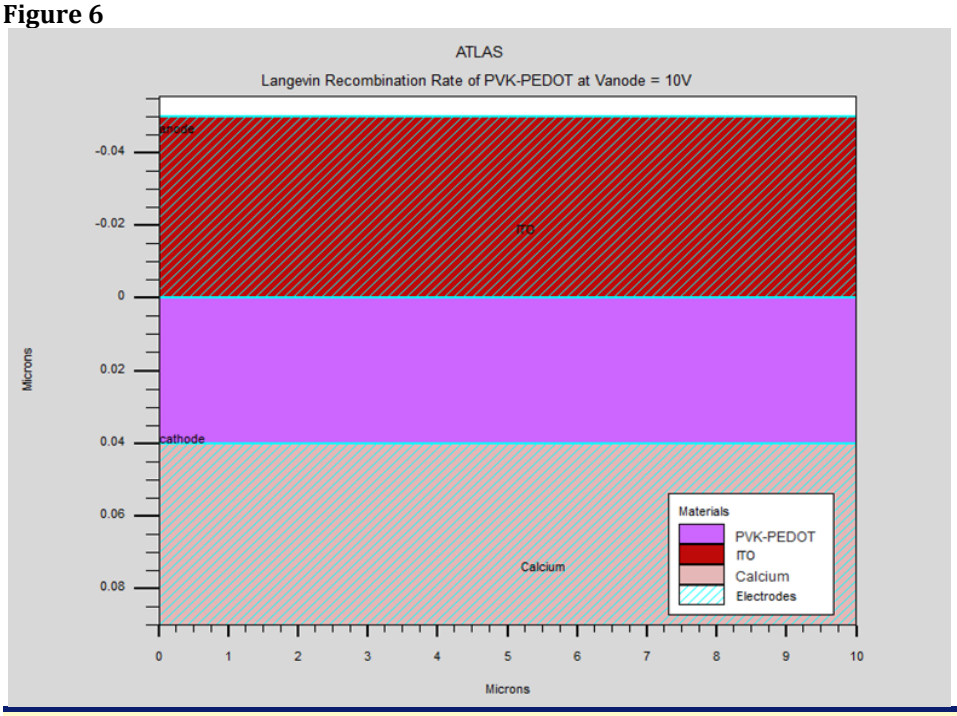

Figure 6 Effect of Active Layer Thickness on Langevin Recombination Rate in OLEDs

6.2. INFLUENCE OF THE THICKNESS

In this study, we investigate the effect of varying the active layer thickness (PVK-PEDOT) on the electrical and optical properties of an organic LED while

maintaining a fixed doping concentration of 1015 cm-3. Figure 6, Figure 7, and Figure 8 show the I-V characteristics, luminescence versus applied voltage, and current versus electric field, respectively, for active layer thicknesses of 40, 60, 80, and 100 nm. The current-voltage (I-V) characteristic reveals that a minimum voltage is required to initiate light emission in an OLED. Our simulation shows that a threshold voltage of 2 volts (VD=2V) is required for a 40 nm active layer. The potential luminescence increases as the anode voltage increases, and the light intensity decreases as the thickness of the emitting layer (PVK-PEDOT) increases. This suggests that reducing the thickness of the active layer leads to improved luminescence and energy efficiency due to reduced direct charge trapping. Therefore, it can be concluded that a thinner emitter layer is preferable.

Figure 7

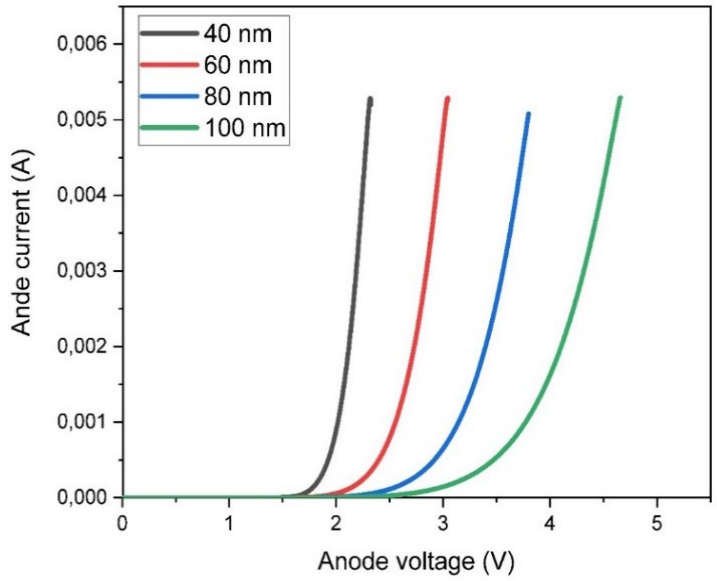

Figure 7 Variations of I-V Characteristics of OLEDs as a Function of Emitting Layer Thickness.

Figure 8

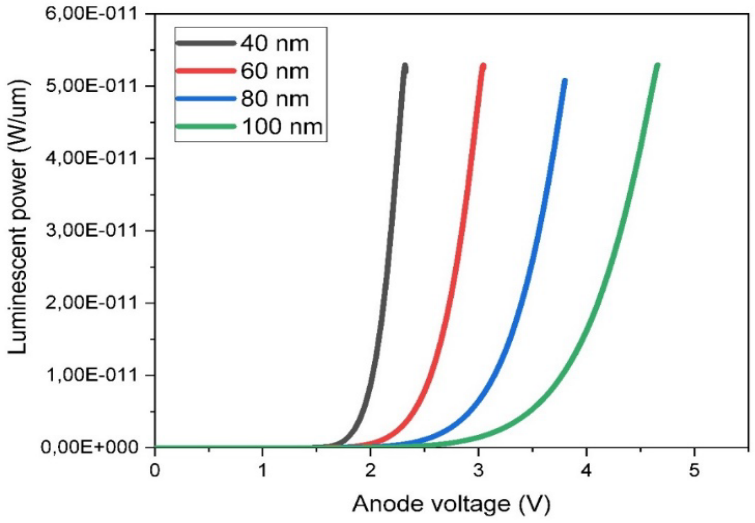

Figure 8 Effect of Emitting Layer Thickness on Luminescent Power as aFunction of Anode Voltage

Figure 9

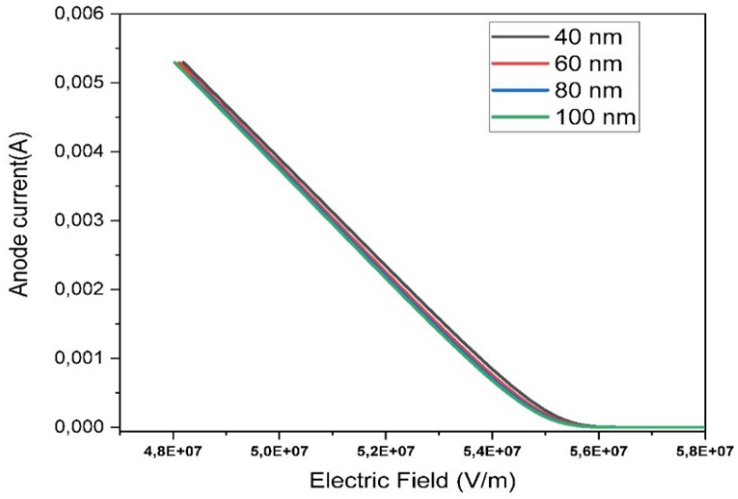

Figure 9 Variation of the Anode Current as a Function of the electric Field for Different Thicknesses of the Active Layer

6.3. INFLUENCE OF CHARGE CARRIER DENSITY

The brightness of OLEDs is directly influenced by the density of the charge carriers, with a higher density resulting in an increase in the brightness of the device. The simulation results, presented in Figure 9, Figure 10, and Figure 11. The results present the I-V characteristics, the variation of luminescence as a function of applied voltage, as well as the evolution of current as a function of electric field for various charge carrier densities in the active layer of an OLED with a constant thickness of 40 nm. The results show that an increase in the anode voltage leads to an increase in the potential luminescence, while an increase in the thickness of the emitting layer (PVK-PEDOT) leads to a decrease in the light intensity. Therefore, it can be concluded that a large value of charge carrier density is beneficial for OLED performance.

Figure 10

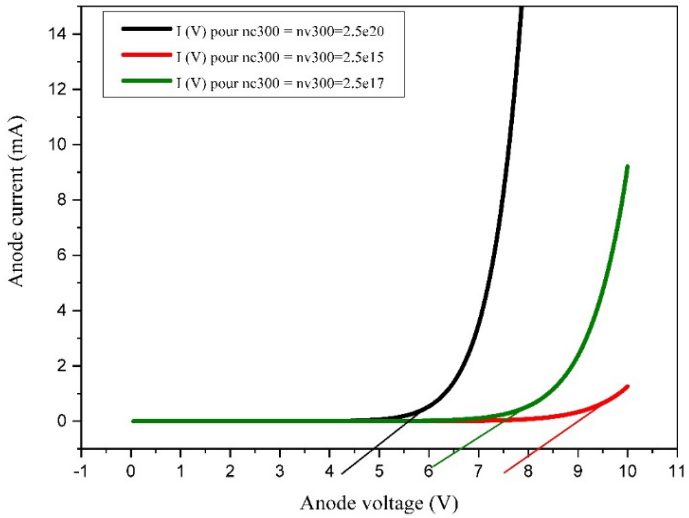

Figure 10 Variations of I-V characteristics of OLEDs as a Function of Charge Carrier Density

Figure 11

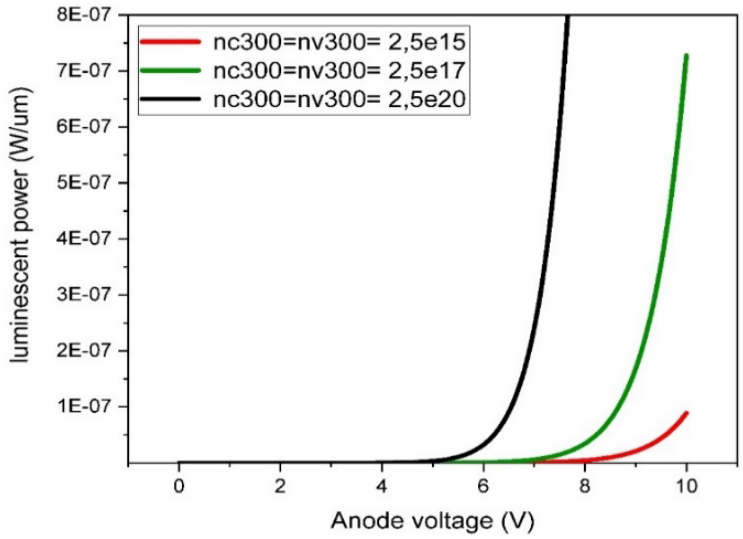

Figure 11 Effect of Charge Carrier Density on Luminescent Power as a Function of Anode Voltage

Figure 12

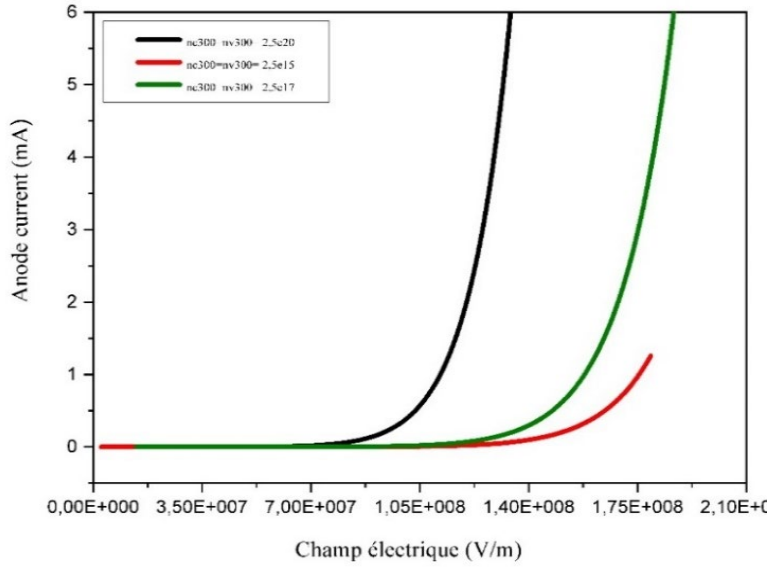

Figure 12 Variation of the Anode Current as a Function of The Electric Field for Different Charge Carrier Density

6.4. INFLUENCE OF TEMPERATURE

In general If temperatures are too high, this can lead to a reduction in screen brightness and a decrease in screen life, while temperatures that are too low can affect screen performance by reducing electron mobility. OLED displays can operate over fairly wide temperature ranges, typically from -20°C to 70°C. Figure 12 shows the I-V characteristics of OLED for different temperature values (280K, 300K, 350K, 380K).

Figure 13

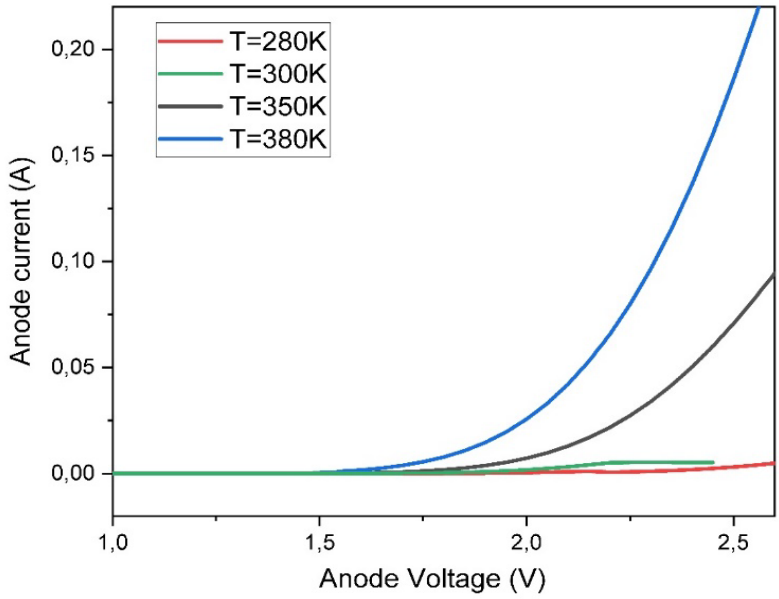

Figure 13 Variations of I-V Characteristics of OLEDs as a Function of Temperature

The threshold voltage, which is the voltage needed to start emitting light, generally increases with increasing temperature and increasing temperature can lead to an increase in the current flowing through the OLED, as it accelerates the mobility of electrons in the organic materials of the OLED. This can lead to an increase in the brightness of the OLED display, but it can also accelerate the degradation of the organic OLED materials and reduce the life of the display. It is therefore important to adhere to the recommended temperature ranges for optimal OLED display operation.

7. CONCLUSION

To predict the electrical and optical properties of an OLED with a PVK-PEDOT emitting layer, Silvaco TCAD software was used in this study. The simulation involved solving the differential equations that describe polymer transport and recombination, as well as determining the radiative rate of luminescence resulting from Langevin recombination in the OLED. The TCAD simulation generated I-V characteristics, voltage-dependent luminescence and electric field-dependent current for different thicknesses and charge carrier densities of the emitting layer, as well as I-V characteristics at different temperatures. The results revealed that reducing the thickness improves the device performance, while high charge carrier density and appropriate temperature ranges are crucial for optimal OLED operation. The simulations provide valuable information about the internal physical processes and help optimize the OLED design, reducing the need for time-consuming and costly experiments on real devices.

CONFLICT OF INTERESTS

None.

ACKNOWLEDGMENTS

None.

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