Scholar Publishing Group
Kinetic Mechanical Engineering
https://doi.org/10.38007/KME.2021.020402
ISSN 2790-2676 Vol. 2, Issue 4: 11-20

Optimization of Solar Cells Based on Finite Volume Method

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Keywords: Finite Volume Method, Solar Cell, Performance Study, Concentration Gradient

Abstract: The interpenetrating network structure between the donor and acceptor materials of a polymeric intrinsic heterojunction photovoltaic cell is formed by nano-scale phase separation, which provides an effective transport channel for exciton diffusion. The aim of this paper is to investigate the performance study and optimization of solar cells based on the finite volume method. This paper investigates the interface and structure/performance optimisation of organic solar cells with the aim of revealing the mechanism of device performance enhancement. Anode modification of organic solar cells based on copper-titanocyanine: fullerene (CuPc: C60) system. To investigate the effect of anode modification on device performance, we introduced CuPc, MoO3, HPCzI and MoO3-doped HPCzI as the anode modification layers of the devices by vacuum vapour deposition. The HPCzI was designed and synthesised in our laboratory and was used as the anode modification for OPV devices for the first time in previous studies. The results show that the device efficiency is maximised when the HPCzI layer doped with 25% MoO3 is used as the anode modification layer. Energy level analysis shows that HPCzI has a better energy level match with ITO, which can improve the hole extraction efficiency. A study of charge transport performance reveals that the doping of HPCzI with MoO3 significantly improves the hole transport capability, which further explains the improved device performance. Active layer modification of organic solar cells based on poly-3-alkylthiophene: fullerene derivatives (P3HT: PC60BM) system. We have prepared p (P3HT) and n (PCBM) modified OPV devices by electrostatic spraying and optimised the p and n layer thicknesses. The results show that the p-modified devices as well as the p- and n-modified devices are more efficient than the devices without any modification. By analysing the charge transport performance of the corresponding single-carrier devices, both p- and n-modified active layers result in increased hole mobility and thus improved device performance. In this paper, the flux difference splitting format (FVM-FDS) based on the finite volume method is combined with the higher-order multistate Riemann solvers (HLL and HLLC), the high-precision reconstruction format (2nd order MUSCL and 5th order WENO) and the total variation-decreasing lunger-Kutta format (TVD-RK) for the 1D ideal MHD problem

(Brio-Wu excitation tube problem), the 2D ideal MHD problem (OrszagTang vortex problem, exploding wave problem, 2D Riemann problem) and 2D resistive MHD problem (double tearing mode instability problem), respectively, a C++ program is written to numerically solve the corresponding set of magnetohydrodynamic equations and obtain simulation results.

1. Introduction

Over the past 10-30 years, scientific researchers have invested a great deal of effort in researching organic solar cells and have made great progress in many aspects such as active materials, device structures and interface modifications. However, in terms of industrialisation, organic photovoltaic solar cells still face many problems, including low photovoltaic conversion efficiency, complex production processes, high costs, poor device stability and lack of flexibility. Therefore, improving device efficiency and finding a process that enables a simple, low-cost, roll-to-roll process is an important research direction for this paper [1-2].

In the study of performance research and optimization of solar cells based on the finite volume method, many scholars have studied it with good results, for example, A X C prepared CuPc: C60 bulk heterojunction stacked devices based on previous studies, using PTCBI/Ag/m-MTDATA as the intermediate connecting layer, and finally obtained an efficiency of 5.7% by adjusting the thickness of each layer [3 Habashi W G found that photoinduced charge transfer from conjugated polymers to fullerenes (C60) is an ultra-fast (within 100 femtoseconds) phenomenon with a much higher rate than the reverse process. This is due to the fact that the conjugation system of C60 surface nodules allows electrons to leave the domain in the molecular orbital consisting of 60 carbon atoms, thus allowing the stabilisation of foreign electrons [4].

In this paper, two aspects of interfacial modification and active layer structure have been investigated from the perspective of optimising the performance of organic solar cells, respectively. The main work carried out includes the following four parts: In the first part, the intrinsic factors of HPCzI and MoO3-doped HPCzI as anode modification layers for organic small molecule solar cells based on the CuPc:C60 system to improve device performance are investigated. In the second part, p- and n-type modified P3HT:PCBM system polymer solar cells (p represents the donor and n represents the acceptor) were prepared based on previous studies of electrostatic spraying in our group, and the thicknesses of the p- and n-type modified and active layers were optimised. The effects of p- and n-type modifications on device performance were investigated through a series of optical and electrical property characterisation. In the third part, we studied the preparation of P3HT:PCBM polymer solar cells with vertical gradient concentration of active layer by electrostatic spraying method, and optimised the thickness of the active layer with gradient concentration, and investigated the effect of gradient concentration of active layer on device performance by a series of optical and electrical characterisation. In the fourth part, a preliminary study on the preparation of polymer solar cell devices based on PTB7:PC70BM system by electrostatic spraying was conducted to find the optimal conditions for the preparation of PTB7:PCBM devices by electrostatic spraying method through the exploration of spraying parameters, device post-treatment and interfacial modification, which laid the foundation for the subsequent research work.

2. Research on the Performance Study and Optimization of Solar Cells Based on the Finite Volume Method

2.1. Substrate Preparation, Cleaning and Pre-Treatment

(1) Substrate preparation

Substrate cleaning is very important in the above-mentioned device preparation process. Because the film thickness is very small in organic solar cells, the flatness and cleanliness of the substrate surface has a great influence on the quality of the film formation and device performance. The steps for substrate preparation are shown in Figure 1.

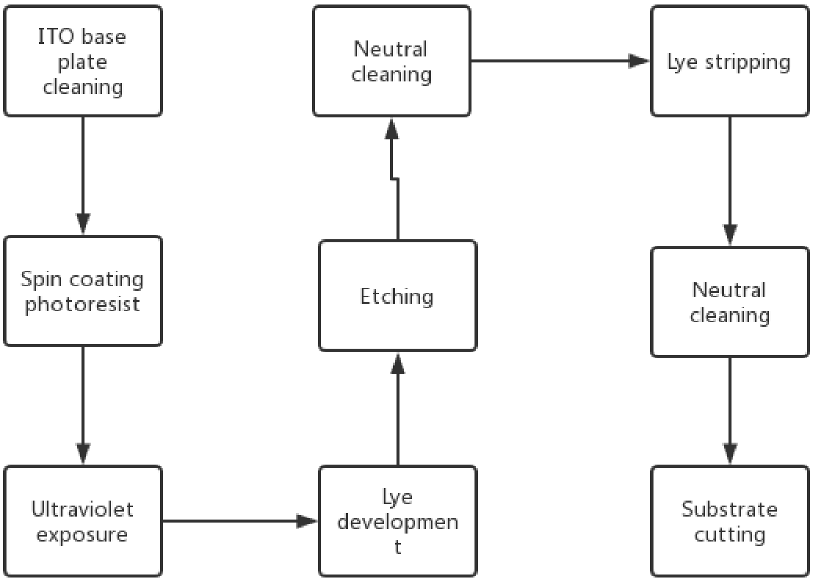

Figure 1. Preparation process of the I T O substrate

(2) Substrate cleaning

The ITO substrates must be cleaned before use as minor contamination of the substrate can affect film formation and therefore device performance. The cleaned substrates were first ultrasonically cleaned using a neutral cleaning solution, TFD7, for 15 min, followed by deionised water, acetone and ethanol for 15 min and finally deionised water for 20 min. The cleaned substrates were dried in a blast oven at 120 ℃ [5-6].

(3) Substrate pre-treatment

In organic solar cells, the surface properties of the device anode ITO have a significant impact on the device. In this thesis, the ITO is pretreated using oxygen plasma treatment, which not only keeps the ITO surface flat, but also improves the work function of the ITO to reduce the hole injection barrier.

2.2. External Quantum Efficiency (Ipce) Testing

The external quantum efficiency (IPCE), also known as incident light conversion efficiency, is the number of electrons per unit incident photon that can be collected by a solar cell (ηEQE). It mainly characterises the spectral response of solar cells to different incident light wavelengths and is important for studying the performance and physical processes of solar cell devices. The external volume efficiency test system used in this laboratory consists of the following main components: light source, monochromator, lens and device test system, lock-in amplifier and PC processing terminal. The test principle of the equipment is to first use a grating monochromator to transform the monochromatic light divided by the light source into alternating monochromatic light of a specific frequency through a modulator, which is irradiated vertically onto a standard compound thin film cell, and the photogenerated current is amplified by a lock-in amplifier to obtain information about the standard sample. The resulting sample is then tested in place of the standard to obtain the device IPCE curve. The phase-locked amplification technique reduces phase and frequency noise during the IPCE test, resulting in high accuracy and precise results [7-8].

2.3. Carrier Mobility

In organic solar cells, carrier transport plays a very critical role in device performance. The magnitude of carrier mobility

It is a form that reflects the ability of charge transport. Mobility is the rate at which a charge can migrate under a given electric field and determines the material

Potential for application in batteries. There are a variety of methods for testing carrier mobility, including field-effect tube analysis, time-of-flight

method, steady-state trap-free space charge-limited current analysis, dark injection space-limited current analysis, transient electroluminescence spectroscopy

analytical methods and time-resolved microwave conduction techniques. Among these methods, the spatially limited current method is a measure of the mobility at a fixed electric field

The more commonly used method. If the effect of trap effects is ignored, the current density can be expressed as the Mott-Gurney equation [9-10].

$$J = \frac{9}{8}\varepsilon_0\varepsilon_r\mu\frac{V^2}{L^3} \quad (1)$$

In this equation, 0 is the vacuum permittivity with a value of 8.85 x 10-12 F/m. ε_r is the relative permittivity. L is the thickness of the sample. μ is the carrier mobility. If the electrodes in the device are in ohmic contact with the material, i.e. in an ideal state, we can directly use the Mott-Gurney equation to find the carrier mobility by squared equation (1) to give [11-12].

$$J^{0.5} = \sqrt{\frac{9\mu\varepsilon_r\varepsilon_0}{8L^3}} * V \quad (2)$$

A linear relationship can be seen between J0.5 and V. A plot of J0.5 as a function of V can be made. When at least one interface is in ohmic contact, the rate of carrier injection is higher than the material's own carrier migration rate at thermal equilibrium, and the concentration of injected carriers is higher than the concentration of its own carriers, the device will exhibit SCLC behaviour. 0.5The slope K can be obtained by a linear fit to this interval [13-14].

3. Research and Design Experiments for the Performance Study and Optimization of Solar Cells Based on the Finite Volume Method

3.1. Cavity Transmission

Cavity transport materials are one of the most important factors affecting the performance of all-solid-state solar cells, and the search for simple, low-cost, environmentally friendly and high-performance cavity transport materials has been a goal pursued by researchers. Organic inorganic layered chalcogenides generally have higher mobility than most organic p-type semiconductors due to their ordered two-dimensional structure [15-16]. To this end, two two-dimensional layered copper chalcogenides, (p-F-C6H5C2H4-NH3)2-CuBr4 and (CH3(CH2)3NH3)2-CuBr4, were prepared in this paper and used as cavity transport materials for the first time in an all-solid-state dye-sensitised solar cell. The Cu-CaTiO3 films prepared by different methods were characterised using ultraviolet-visible absorption (UV/Vis) and X-ray diffraction (XRD), the cell efficiency was tested, and impedance analysis of the cells was performed to explore the effect of Li-TFSI and TBP on the doping of Cu-CaTiO3 cavity transport materials on device performance [17-18].

3.2. Experimental Design

In this paper the performance of solar cells based on the finite volume method is investigated, firstly by comparing the parameters of the cells prepared with different modification materials. The analysis of each parameter and the iv-curves are compared with each other. In fact, the electrochemical impedance spectra are analysed.

4. Experimental Analysis of Research on the Performance Study and Optimization of Solar Cells Based on the Finite Volume Method

4.1. Comparison of Battery Parameters

In this paper, two different modified materials were selected to do a comparison of the corresponding individual parameters and the main experimental data are shown in Table 1. The conclusions drawn are the same as those derived from the curves in Figure 2.

Table 1. Comparison of the parameters of organic photovoltaic cells prepared with different cathode-modified materials

	Voc	Jsc	FF	PCE
LiF	0.71	6.8	31.3	1.51
CF_3 COOCs	0.43	2.1	33.9	0.31

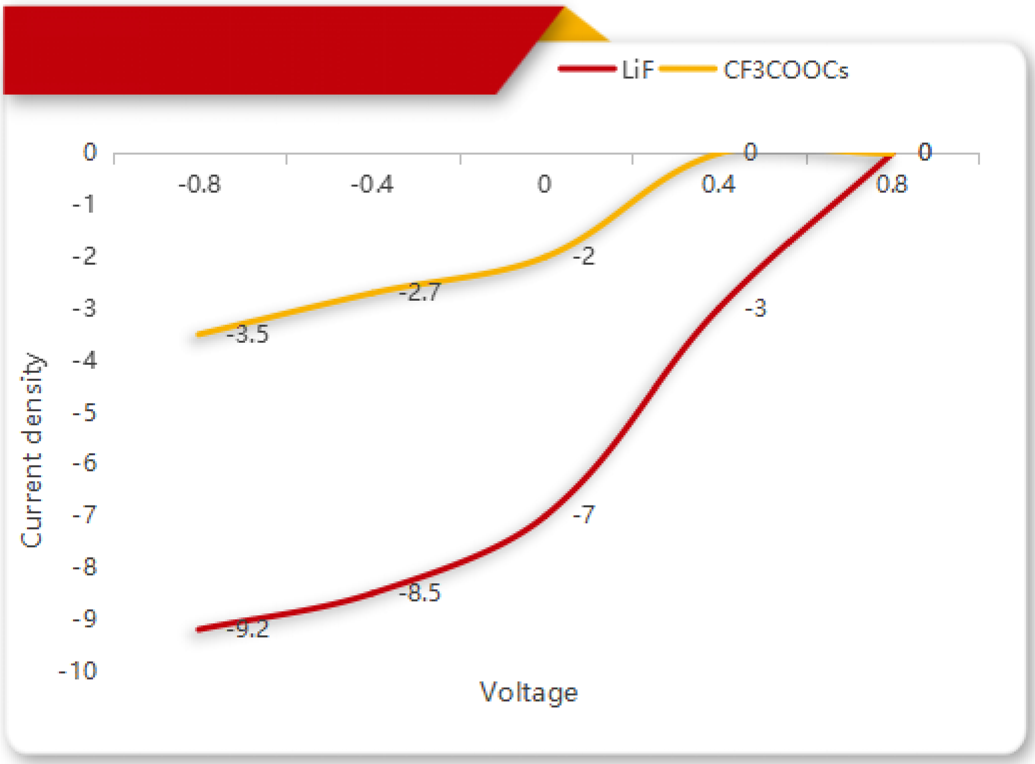

Figure 2. Comparison of the J-V curves of organic photovoltaic cells prepared with different cathode-modified materials

From the comparison of I-V curves of organic PV cells prepared with different cathode modification materials in Fig. 2, it can be seen that cesium trifluoroacetate does not exhibit good cathode modification, which reduces the performance of organic PV cells compared to conventional LiF.

4.2. Electrochemical Impedance Spectroscopy

In order to analyse the effect of the internal resistance of the cell on the performance of the device, electrochemical impedance tests were carried out on the device. The impedance plots for the gradient concentration and each optimum thickness of the P3HT: PCBM device are shown in Figure 3. The intercept of the high frequency region section with the X-axis is the series resistance of the device and this resistance represents the efficiency of charge transfer in the device. The simulated equivalent circuit is the same as for the p- and n-modified devices.

Figure 3 shows the impedance information of the devices obtained by comparing the gradient concentration and the optimum thickness of the P3HT: PCBM devices. The impedance spectrum of the device is semi-circular as can be seen from the figure. The equivalent circuit model we have chosen is the same as in Chapter 4. By using this equivalent circuit to fit the device impedance spectrum, specific parameter values for the series resistance (Rs), the charge transfer resistance of the active layer (RBulk) and the bimolecular composite resistance (RRec) can be obtained, as shown in Table 2. The lower Rs indicates more effective charge collection in the gradient-concentration devices, which corroborates the J-V curve findings above.

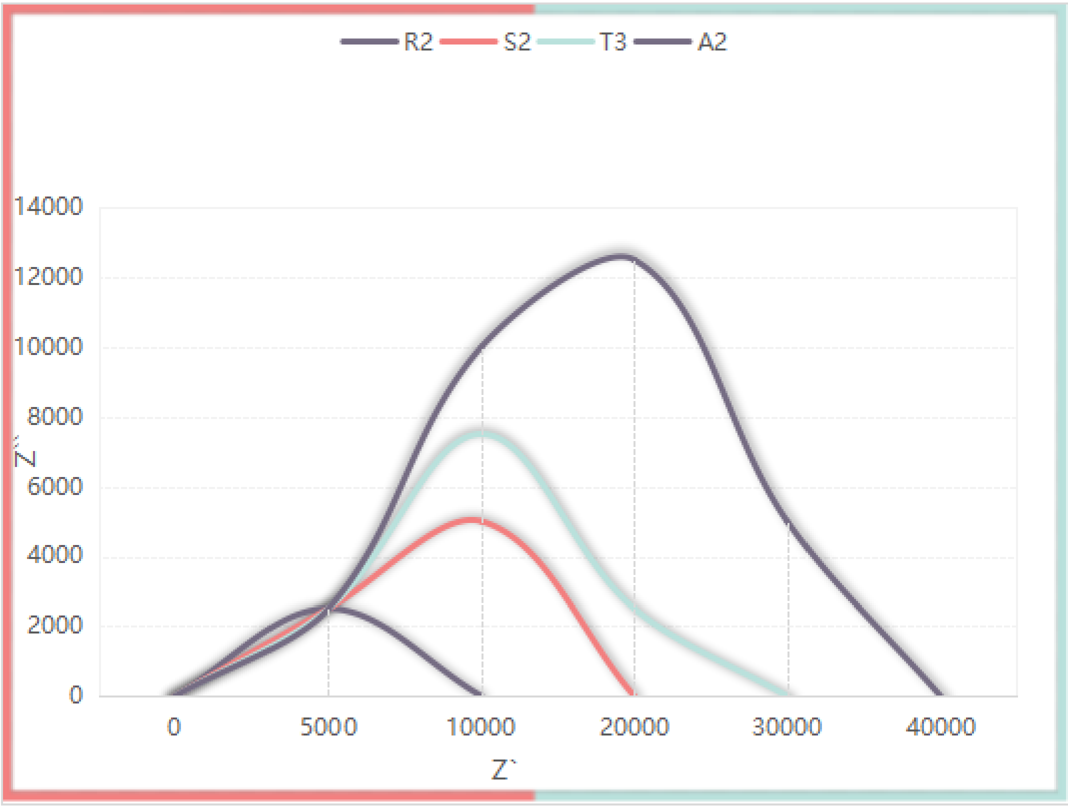

Figure 3. Gradient concentration and P3HT: The impedance spectrum of the best thickness device of PCBM

Table 2. equivalent circuit simulation parameters table

	Rs	C1	Rbulk	C2	Rrec	Error
R2	4.883	7.496E-8	3300	2.197E-6	2544	2.65E-4
S2	5.855	8.549E-8	5340	1.547E-8	2030	1.42E-3
T3	5.404	7.42E-8	1469	9.304E-7	1.509E4	4.1E-4
A2	7.076	6.982E-8	2.054E4	7.535E-8	1.634E4	4.25E-3

5. Conclusion

This paper briefly investigates the effect of interfacial modification on small molecule organic solar cells based on the finite volume method, focusing on the effect of active layer modification and structural optimization on the performance of polymer solar cells, and briefly explores the preparation conditions for the preparation of devices based on the PTB7:PCBM system using the electrostatic spray method. The details are as follows: (1) CuPc, HPCzI, MoO3 and HPCzI doped with 25% and 50% MoO3 were used as the anode interface modification layer for the CuPc:C60 system based devices, and the HPCzI devices showed an improved efficiency of 1.62% compared to the CuPc and MoO3 devices. When doped with 25% MoO3, the PCE increases to 1.71%. The analysis for energy level and charge transport properties reveals that HPCzI can match better with ITO, which is more conducive to hole extraction and reduces charge compounding. By doping HPCzI with MoO3, the hole mobility of the device is significantly improved by 3-4 orders of magnitude compared to CuPc and HPCzI devices. The fundamental reason for the improved device efficiency was found. (2) Organic solar cells based on P3HT:PCBM active layer were prepared by electrostatic spray method, and the relationship between active layer thickness and device performance of bulk heterojunction devices was explored. The results showed that the device PCE was highest at 100 nm active layer thickness, reaching 2.43%. Based on the above investigation, p- and n-type modified devices based on the P3HT:PCBM system were designed, and the receptor and donor materials were sprayed alternately on the top and bottom of the active layer by electrostatic spraying method. By optimising the thickness of each p- and n-type layer, it was found that the p-type modification had a 7% improvement in PCE compared to the P3HT:PCBM device at a thickness of 13 nm, reaching 2.49%. However, the n-type modification resulted in a significant reduction in JSC and an increase in VOC, but did not improve device efficiency. When both p and n modified the active layer, the current increased compared to the n-type modified device, and VOC also increased, improving the efficiency to 2.53%. To investigate the reasons for the increased efficiency, the optical properties of the films as well as the electrical properties of the devices were explored. The UV-visible absorption peaks of the p-type modified films were found to be more pronounced at 550nm and 600nm, with a slight increase in device IPCE and a smaller Rs. The hole mobility was larger than that of the n-type modification, and the hole mobility was greatest when both p and n types were modified. This indicates that p-type modification can improve the hole transport of OPV devices, and n-type modification can greatly improve the VOC although it is not conducive to hole transport, so p and n simultaneous modification improves the overall performance of OPV devices. (3) P3HT:PCBM-based organic solar cells with vertical gradient concentration were prepared by electrostatic spraying, and the top and bottom of the active layer were alternately sprayed with the receptor enrichment layer and the feeder enrichment layer: PCBM devices showed a 61% improvement in PCE. However, the addition of a receptor enrichment layer D:A<1:0.8 resulted in a significant reduction in JSC and did not improve device efficiency.

Funding

This article is not supported by any foundation.

Data Availability

Data sharing is not applicable to this article as no new data were created or analysed in this study.

Conflict of Interest

The author states that this article has no conflict of interest.

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