

# An analysis for S-shaped $I$ - $V$ characteristics of organic solar cells using lumped-parameter equivalent circuit model

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## ABSTRACT

A lumped-parameter equivalent circuit model of organic solar cells (OSCs) is proposed to analyze the S-shaped current-voltage ( $I$ - $V$ ) characteristics and the explicit solution to  $I$ - $V$  equation is derived so that this model is suitable to be compactly implemented for the simulations of photovoltaic applications. Comparing our explicit solutions with the method of least squares and the Newton-Raphson root-finding scheme, the simulations quantitatively reproduce the S-shaped  $I$ - $V$  characteristics of OSCs especially for both linear- and exponential-like S-shaped kink in the third and first quadrants, respectively. Simultaneously, the simulations facilitate us to qualitatively analyze the S-shaped  $I$ - $V$  characteristics of OSCs influenced by the different model parameters. Furthermore, we verify the simulation results of our proposed model by using the reconstructed experimental data. Good agreements indicate that such a model can be used to accurately predict the S-shaped  $I$ - $V$  characteristics of OSCs and regarded as a serviceable tool implemented compactly into simulations of the wide photovoltaic applications.

## 1. Introduction

Today, electronic devices are facing a disruptive evolution, developing from heavy and rigid appliances to light and flexible devices. As the most promising next generation electronic devices, organic devices, such as organic thin-film transistors (OTFTs) and organic solar cells (OSCs), are mainly intended for low-cost, large-area, and flexible applications. Up to date, OSCs are still in the intensive researches (Tran et al., 2017; Sanchez et al., 2017; Dominguez et al., 2017) for suppressing S-shaped  $I$ - $V$  characteristics (Wagenpfahl et al., 2010) to achieve high power-conversion efficiency (PCE) comparable to the conventional silicon-based solar cells (Chavali et al., 2017; Kale and Solanki, 2015; Yoshikawa et al., 2017). Therefore, an important requirement for the OSC applications in the engineering field is to have lumped-parameter equivalent circuit models that can be compactly implemented into simulators to predict and optimize the performances of OSCs.

The operating principle of OSCs is qualitatively similar as that of silicon-based solar cells, but the anomalous S-shaped kink observed in OSCs'  $I$ - $V$  characteristics impairs the J-shaped  $I$ - $V$  curve and PCE. Because the earlier conventional lumped-parameter models (Ortiz-Conde et al., 2014) including single diode failed in describing the S-shaped kink, multiple-diode lumped-parameter models (Mazhari, 2006;

De Castro et al., 2010; Zuo et al., 2014; Kumar and Gaur, 2013; Gaur and Kumar, 2014; García-Sánchez et al., 2013; De Castro et al., 2016; Roland et al., 2016; Xu et al., 2018; Huang et al., 2018) are proposed to give some reasonable explanations on it from the view of electricity. Mazhari (2006) understood the incapacity of single-diode models in describing the S-shaped kink and suggested that two more diodes are used to produce the non-constant photo-current and concave S-shaped behavior, respectively. Up to now, Mazhari's model (Mazhari, 2006) is the simplest circuit in all of the above three-diode models because the least fitting parameters are required for simulations. Of course, the improvement rooms on efficiency and accuracy of computing Mazhari's model are still left for us. B. Mazhari's model (Mazhari, 2006) is unable to model the linear-like rise S-shaped kink in the third quadrant due to the absence of resistance Xu et al. (2018) and Huang et al. (2018). De Castro et al. (2010) and Zuo et al. (2014) proposed two-diode lumped-parameter models, which cannot demonstrate Heterojunction OSCs' S-shaped kink with the exponential-like rise in the first quadrant. Kumar and Gaur (2013) and Gaur and Kumar (2014) proposed two improved equivalent circuit models to represent the behavior of polymer solar cells under different environmental conditions, but these two models do not result in a compact formulation. García-Sánchez et al. (2013) dealt with the inability of F. Araujo de Castro's model by adding another diode, which allows the experimentally observed exponential-like

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upturn but not linear-like upward bend of the illuminated  $I$ - $V$  characteristics in the first quadrant. Subsequently, to seek further generalization, De Castro et al. (2016) and Roland et al. (2016) published the corresponding modifications of the previous model (García-Sánchez et al., 2013) to gain insight into the modelling and parametrization of OSC current-voltage curves. In general, it is not mathematically possible to obtain an analytical solution to the above two models (De Castro et al., 2016; Roland et al., 2016). Therefore, numerical iteration or approximate methods are commonly used to solve the above two models, where numerical iteration solutions consume much computation time and approximate method solutions easily reduce computation accuracy. Finally, Xu et al. (2018) and Huang et al. (2018) improved B. Mazhari's model to simulate the linear-like S-shaped kink probably existing in the third quadrant.

The fundamental novelty of this paper is proposing an improved three-diode lumped-parameter equivalent circuit model of OSCs. Such a model can visualize the overall shape of the S-shaped  $I$ - $V$  characteristics, thus facilitating us to give further researches on underlying physical phenomena of OSCs. The immediate contribution of this paper is deriving the explicit solution of the proposed model to avoid the need for numerical iteration or approximate method solutions to express the OSCs' electrostatic performance. The explicit solutions to our model help to easily extract the fitting parameters, significantly speed up the process of simulating OSCs'  $I$ - $V$  characteristics, and promptly analyze the effects from the model parameters. Finally, the method of least squares, Newton-Raphson root-finding scheme, and the measured  $I$ - $V$  data of OSCs validate the explicit solution to our proposed model. Good verification results illustrate that our proposed model can accurately reproduce the S-shaped  $I$ - $V$  plots of OSCs and the derived explicit solution can implement compactly our model into simulations of OSCs' applications.

## 2. Proposed lumped-parameter model of organic solar cells

The previous lumped-parameter equivalent circuit model proposed by Mazhari (2006) includes only six parameters resulting from three diodes, as shown in Fig. 1. Compared with inorganic solar cells, excitons instead of free carriers are created in organic solar cells (OSCs). These excitons subsequently diffuse to the interface between donor and acceptor films and dissociate to form polaron-pairs. After the generation of polaron-pairs, they either recombine to form recombination current  $I_R$  or be extracted by electrodes to form extraction current  $I_E$ . In addition,  $I_D$  is the dark current of the device in the absence of light. For a given light intensity,  $I_{ph}$  is the current representing the polaron-pair generation rate.  $I$  and  $V$  are the terminal current and voltage of the OSCs, respectively. In fact, the terminal current depends on competition between polaron recombination and its collection by the electrodes. Because the free charge collection or extraction efficiency depends on internal electric field, it is expected that current would, in general, depend on voltage across the device.

In Mazhari's model, as shown in Fig. 1, current source  $I_{ph}$  demonstrates the net polaron generation rate, which is a constant in the case of a fixed light intensity. The diodes,  $D_R$ ,  $D_E$ , and  $D_D$  model the loss of

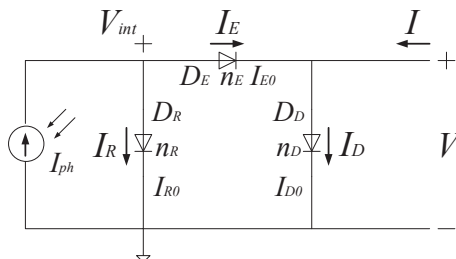


Fig. 1. The organic solar cells' lumped-parameter equivalent circuit model (Mazhari, 2006) proposed by B. Mazhari.

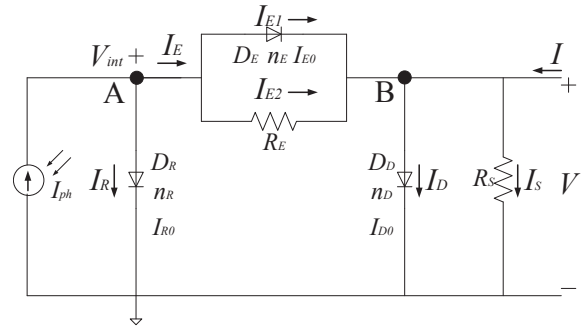


Fig. 2. The improved lumped-parameter equivalent circuit model of organic solar cells.

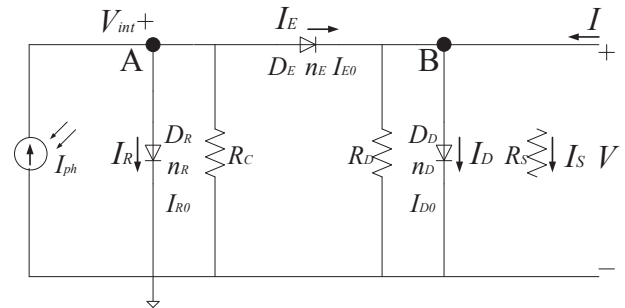


Fig. 3. The equivalent lumped-parameter circuit with Fig. 2 according to Miller theorem.

polarons due to recombination, the extraction due to internal electric field, and the  $I$ - $V$  characteristics of the OSCs in the absence of light, respectively. Mazhari's model can both qualitatively and quantitatively analyze the electrical properties of OSCs, especially for the S-shaped  $I$ - $V$  characteristics. It is noted that there are not any series or shunt resistances in Mazhari's model. As a result, the simulations of Mazhari's model for OSCs are not enough accurate in the first and third quadrants (Xu et al., 2018; Huang et al., 2018).

In this paper, we improve Mazhari's model by adding two shunt resistances  $R_E$  and  $R_s$  as shown in Fig. 2. From mathematical aspects, the shunt resistances  $R_E$  and  $R_s$  are used to improve the accuracy of the simulations for OSCs' S-shaped  $I$ - $V$  characteristics. From physical aspects, both  $D_E$  and  $R_E$  instead of only  $D_E$  model the extraction current  $I_E$  of free carriers following the dissociation of polarons. In addition,  $R_s$  is used to describe the parasitic resistance in OSCs.

From circuit aspects, according to Miller theorem, the lumped-parameter circuit in Fig. 2 can be transformed into the following circuit as shown in Fig. 3. However, two more shunt resistances  $R_C = \frac{V_{int} \cdot R_E}{V_{int} - V}$  and  $R_D = \frac{V \cdot R_E}{V_{int} - V}$  are added into Mazhari's model. Obviously, the lumped-parameter equivalent circuit model of OSCs including only two shunt resistances in Fig. 2 is simpler than that in Fig. 3. Simultaneously, the circuit in Fig. 2 also assures the accuracy of simulations for OSCs' S-shaped characteristics.

## 3. Model's equation explicit solution

Our improved lumped-parameter equivalent circuit by adding  $R_E$  is to predict accurately the S-shaped  $I$ - $V$  characteristics of OSCs, as shown in Fig. 2. At points A and B, applying Kirchhoff's current law to the circuit of Fig. 2, we can obtain

$$I_{ph} = I_R + I_E, \quad (1)$$

$$I = I_D + I_S - I_E. \quad (2)$$

Subsequently, we substitute the standard diode equation (Shockley, 1949) into (1) and (2), yielding

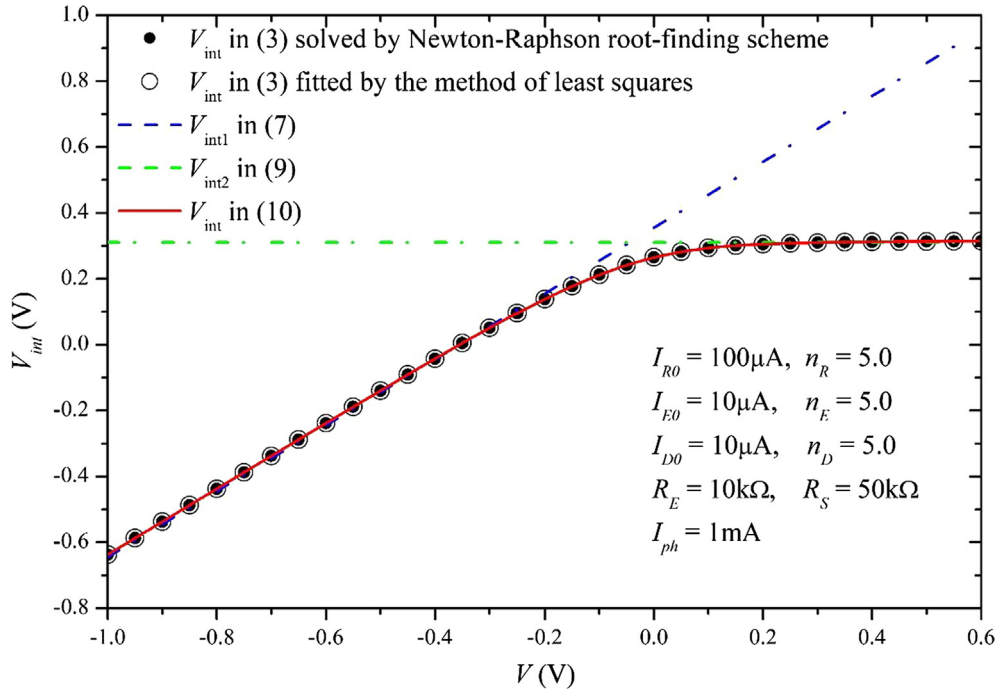


Fig. 4.  $V_{int}$  vs.  $V$  in our equivalent lumped-parameter circuit of Fig. 2.

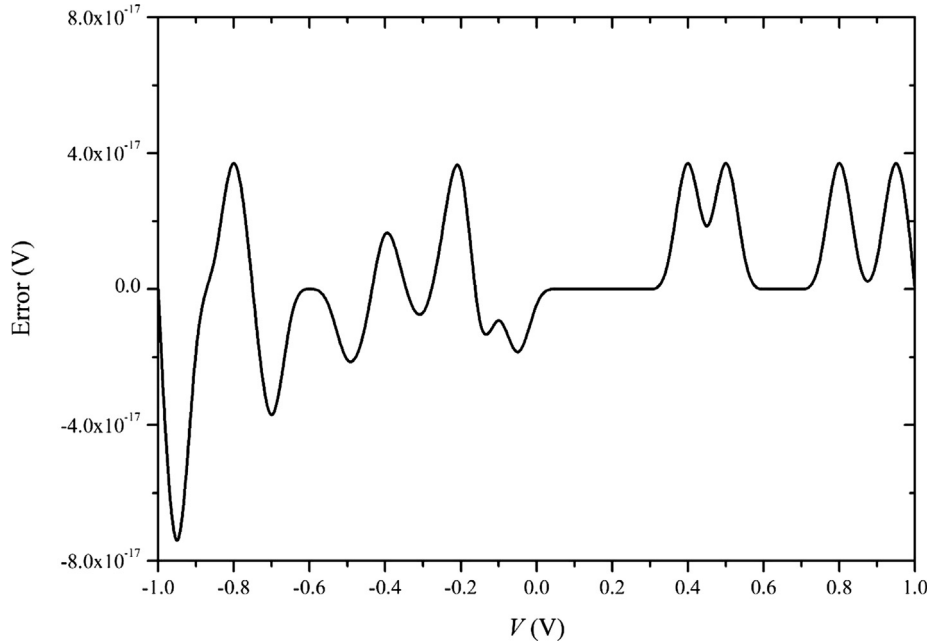


Fig. 5. Errors between  $V_{int}$  calculated in (10) and  $V_{int}$  in (3) fitted in the method of least squares.

$$I_{ph} = I_{R0} \left( e^{\frac{V_{int}}{n_R V_t}} - 1 \right) + \left[ I_{E0} \left( e^{\frac{V_{int}-V}{n_E V_t}} - 1 \right) + \frac{V_{int}-V}{R_E} \right], \quad (3)$$

$$I = I_{D0} \left( e^{\frac{V_{int}}{n_D V_t}} - 1 \right) + \frac{V}{R_S} - \left[ I_{E0} \left( e^{\frac{V_{int}-V}{n_E V_t}} - 1 \right) + \frac{V_{int}-V}{R_E} \right]. \quad (4)$$

If we look forward to solving the  $I$ - $V$  characteristics of OSCs, combining (3) and (4) to eliminate  $V_{int}$  is necessary for deriving the relationship between  $I$  and  $V$ , which is also the transcendental function (Romero et al., 2017). This process is too complicated to solve analytically the expression  $I$  as a function of  $V$ . Of course, in our previous works (Xu et al., 2018; Huang et al., 2018), we avoid to directly solve the expression of  $I$  from the transcendental function. On the contrary,

we firstly derive  $V_{int}$  from (3) through the Newton-Raphson root-finding method, and then we secondly substitute the results of  $V_{int}$  into (4) to obtain the  $I$ - $V$  characteristics of OSCs. After all, the Newton-Raphson root-finding method is a kind of numerical iteration method, which consumes amount of computational time, leading to the poor computational efficiency. In this paper, in order to improve the computational efficiency, we analytically derive the expression of  $V_{int}$  from (3) through the regional approach, which is to be shown as follows.

In the case of backward terminal voltage  $V$ , the internal electric field existing in OSCs collects and extracts the free charges resulting from polaron-pairs. From the view of physical significance, in Fig. 2, the extraction current  $I_E$  is much larger than the recombination current  $I_R$ . From the view of mathematical computation, in (3),

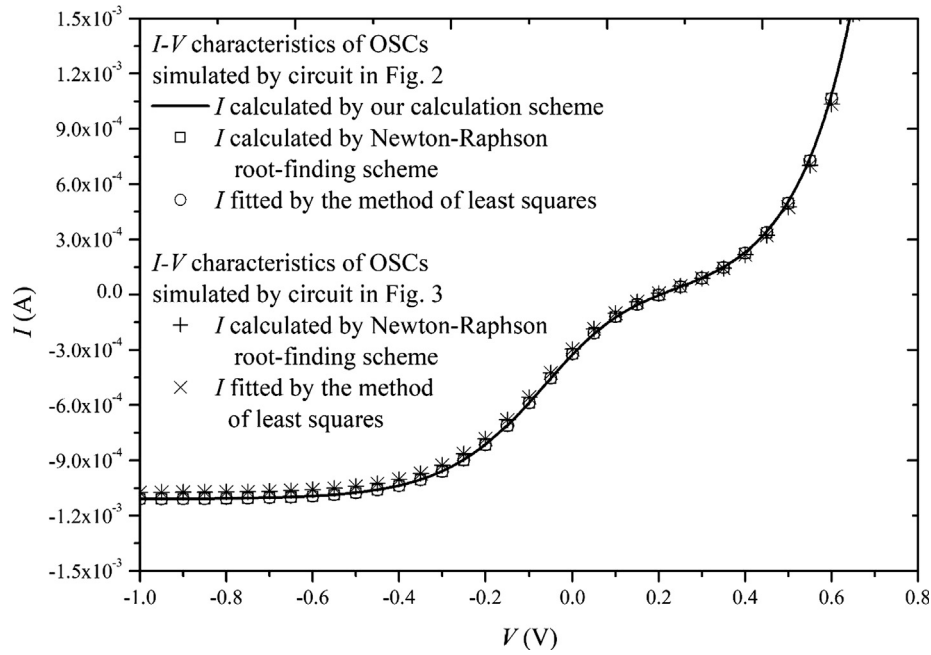


Fig. 6.  $I$  vs.  $V$  simulated by lumped-parameter circuits in Figs. 2 and 3.

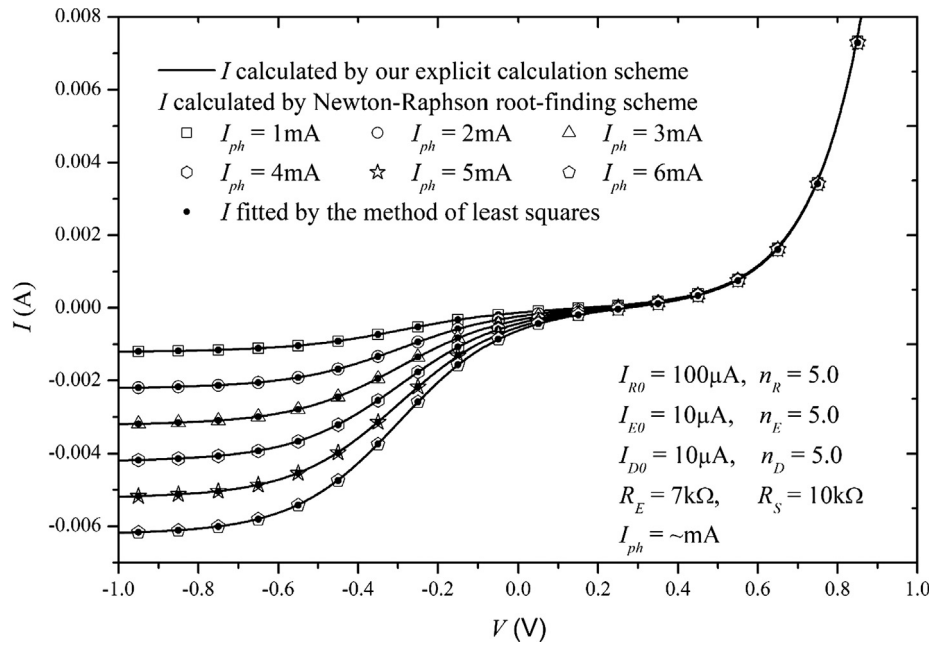


Fig. 7. Effects from  $I_{ph}$  on  $I$ - $V$  characteristics of OSCs simulated by our lumped-parameter circuits.

representing  $I_E$  is the dominant item in the right hand side (RHS) of (3). Considering the condition that  $\left[ I_{E0} \left( e^{\frac{V_{int}-V}{n_E V_t}} - 1 \right) + \frac{V_{int}-V}{R_E} \right] \gg I_{R0} \left( e^{\frac{V_{int}}{n_R V_t}} - 1 \right)$ , we can simplify (3) as

$$I_{ph} = I_{E0} \left( e^{\frac{V_{int1}-V}{n_E V_t}} - 1 \right) + \frac{V_{int1}-V}{R_E}. \quad (5)$$

Here,  $V_{int1}$  is the asymptotic solution of  $V_{int}$  in (3). It is noted that (5) is only valid for the case of large backward terminal voltage  $V$ , because we neglect the item  $I_{R0} \left( e^{\frac{V_{int}}{n_R V_t}} - 1 \right)$  in (3). Now, only one exponent item is included in (5). Therefore, we can reformulate (5) as the typical mathematical formula of the Lambert  $W$  function (Corless et al., 1996), i.e.,

$$\left[ \frac{R_E (I_{ph} + I_{E0})}{n_E V_t} - \frac{V_{int1} - V}{n_E V} \right] \cdot \exp \left[ \frac{R_E (I_{ph} + I_{E0})}{n_E V_t} - \frac{V_{int1} - V}{n_E V_t} \right] = \frac{R_E I_{E0}}{n_E V_t} \cdot \exp \left[ \frac{R_E (I_{ph} + I_{E0})}{n_E V_t} \right]. \quad (6)$$

Furthermore, we can derive the expression of  $V_{int1}$  from (6) as

$$V_{int1} = V + R_E (I_{ph} + I_{E0}) - n_E V_t \cdot W_0 \left[ \frac{R_E I_{E0}}{n_E V_t} \cdot \exp \left( \frac{R_E (I_{ph} + I_{E0})}{n_E V_t} \right) \right]. \quad (7)$$

Here,  $W_0$  is the Lambert  $W$  function's principal branch (Corless et al., 1996), as a typical solution to equation  $W_0(x)e^{W_0(x)} = x$ .

In the case of forward terminal voltage  $V$ , the internal electric field existing in OSCs is not enough strong to collect polaron-pairs by two electrodes, i.e., anode and cathode. From the view of physical

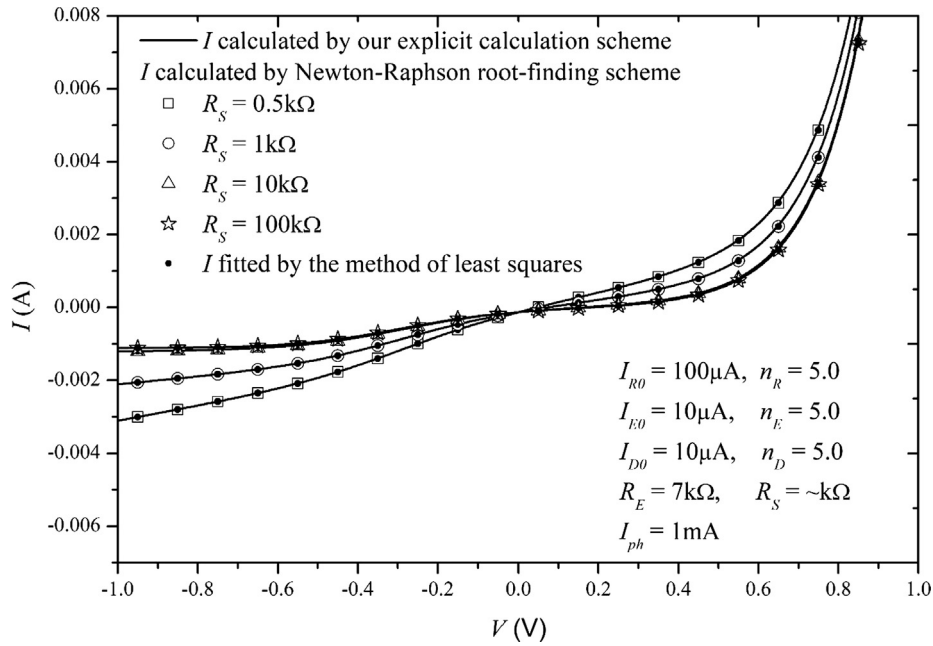


Fig. 8. Effects from  $R_S$  on  $I$ - $V$  characteristics of OSCs simulated by our lumped-parameter circuits.

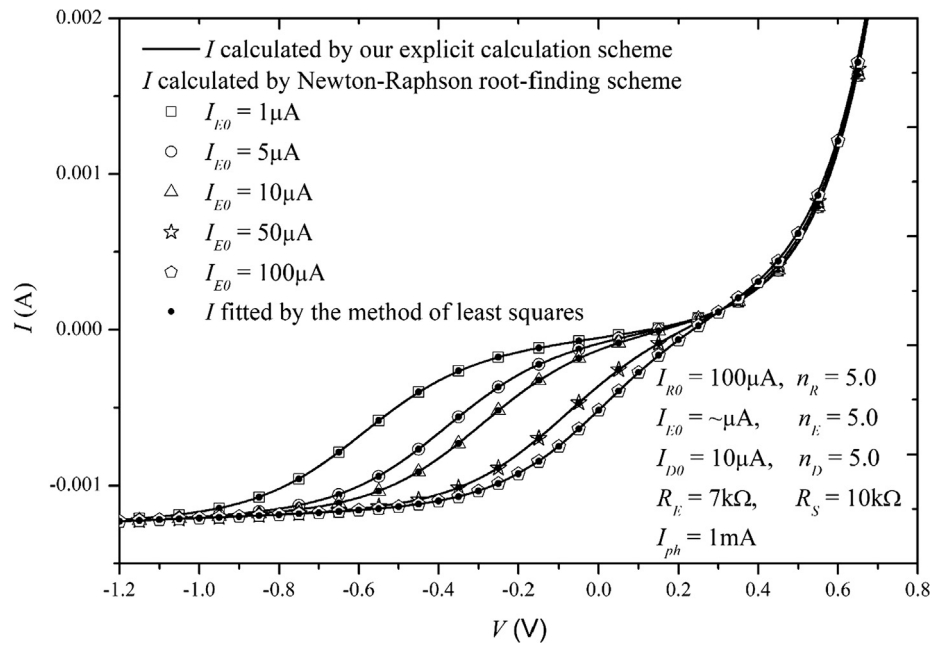


Fig. 9. Effects from  $I_{E0}$  on  $I$ - $V$  characteristics of OSCs simulated by our lumped-parameter circuits.

significance, in Fig. 2,  $I_R$  is much larger than  $I_E$ . From the view of mathematical computation,  $I_{R0} \left( e^{\frac{V_{int}}{n_R V_t}} - 1 \right)$  is the dominant item in the RHS of (3). Considering the condition that  $I_{R0} \left( e^{\frac{V_{int}}{n_R V_t}} - 1 \right) \gg \left[ I_{E0} \left( e^{\frac{V_{int}-V}{n_E V_t}} - 1 \right) + \frac{V_{int}-V}{R_E} \right]$ , we can simplify (3) as

$$I_{ph} = I_{R0} \left( e^{\frac{V_{int2}}{n_R V_t}} - 1 \right). \quad (8)$$

Here,  $V_{int2}$  is the asymptotic solution of  $V_{int}$  in (3). It is noted that (8) is only valid for the case of forward terminal voltage  $V$ , because we neglect the item  $\left[ I_{E0} \left( e^{\frac{V_{int}-V}{n_E V_t}} - 1 \right) + \frac{V_{int}-V}{R_E} \right]$  in (3). We can derive the expression of  $V_{int2}$  from (8) as

$$V_{int2} = n_R V_t \cdot \ln \left( \frac{I_{ph}}{I_{R0}} + 1 \right). \quad (9)$$

In order to obtain the results of  $V_{int}$  valid for the whole operational region of OSCs (i.e., including both backward and forward terminal voltage  $V$ ), we use the smoothing function to connect the expressions  $V_{int1}$  and  $V_{int2}$  and Schrodter series to improve the accuracy of  $V_{int}$ , yielding

$$V_{int} = \frac{1}{10} \cdot \ln \left[ \frac{1}{1/\exp(10 \cdot V_{int1}) + 1/\exp(10 \cdot V_{int2})} \right] + \omega. \quad (10)$$

Here, we modify the starting function  $V_{int}$  in (10) by adding the correction of Schrodter series  $\omega$  (Deng et al., 2014; Yu et al., 2016), which is symbolled as  $\omega = (y/y')/(1 - 0.5y''/y')$ , where



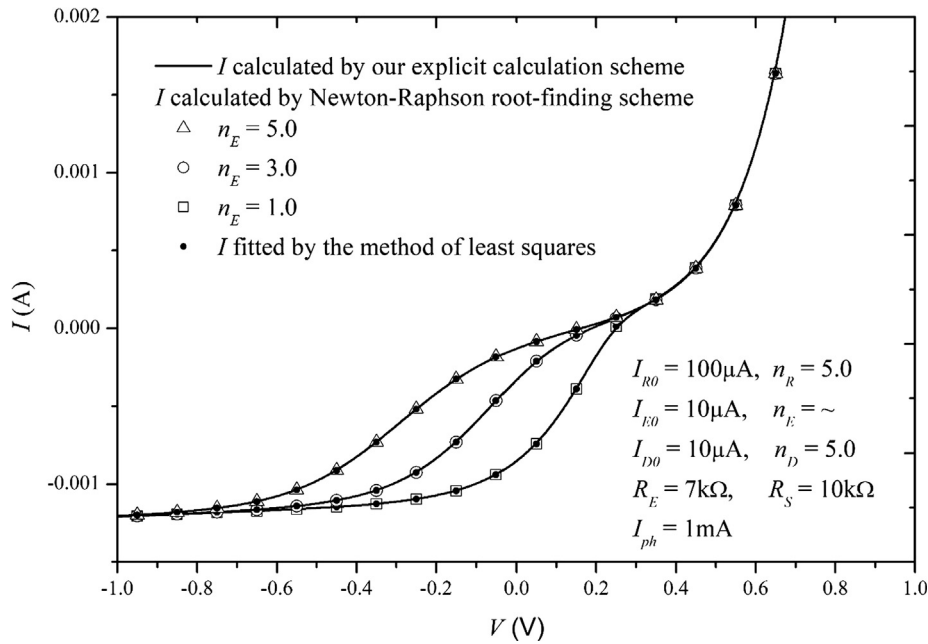


Fig. 10. Effects from  $n_E$  on  $I$ - $V$  characteristics of OSCs simulated by our lumped-parameter circuits.

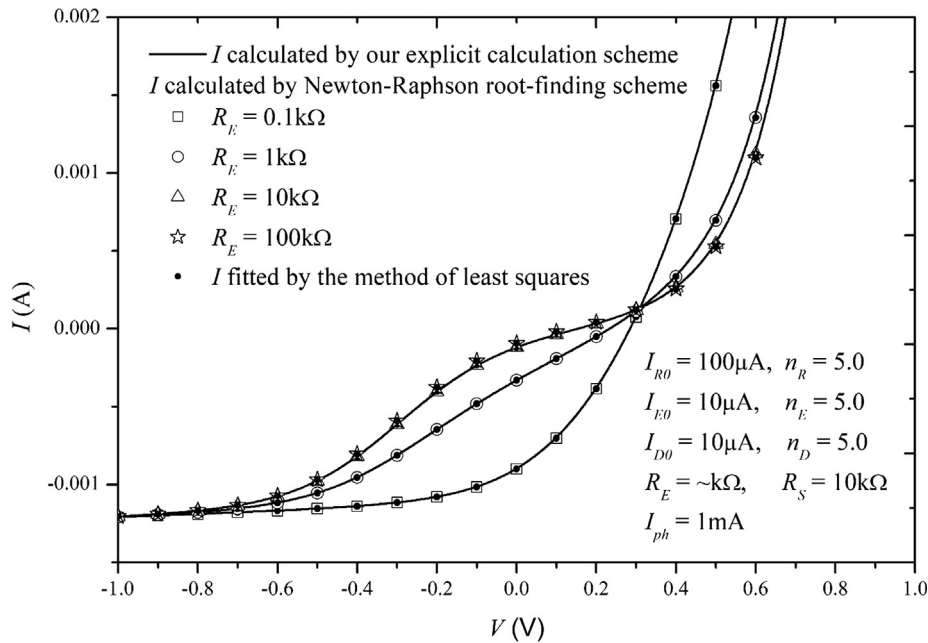


Fig. 11. Effects from  $R_E$  on  $I$ - $V$  characteristics of OSCs simulated by our lumped-parameter circuits.

$y = I_{R0} \left( e^{\frac{V_{int}}{n_R V_t}} - 1 \right) + \left[ I_{E0} \left( e^{\frac{V_{int}-V}{n_E V_t}} - 1 \right) + \frac{V_{int}-V}{R_E} \right] - I_{ph}$ ,  $y'$  is the first derivative of  $y$  versus  $V_{int}$  with  $y' = \frac{I_{R0}}{n_R V_t} \cdot e^{\frac{V_{int}}{n_R V_t}} + \frac{I_{E0}}{n_E V_t} \cdot e^{\frac{V_{int}-V}{n_E V_t}} + \frac{1}{R_E}$ , and  $y''$  are the second derivative of  $y$  versus  $V_{int}$  with  $y'' = \frac{I_{R0}}{(n_R V_t)^2} \cdot e^{\frac{V_{int}}{n_R V_t}} + \frac{I_{E0}}{(n_E V_t)^2} \cdot e^{\frac{V_{int}-V}{n_E V_t}}$ . In fact, the method that deriving the starting function and then modifying it with Schroder series has been regarded as a universal fashion (Deng et al., 2014; Yu et al., 2016).

In Fig. 4, we show  $V_{int1}$ - $V$ ,  $V_{int2}$ - $V$ , and  $V_{int}$ - $V$  characteristics. According to analysis of (7),  $V_{int1}$  is only suitable for the case of backward terminal voltage  $V$ . That is consistent with the results of  $V_{int}$  on the condition that  $V < 0$  V, as shown in Fig. 4. According to analysis of (9),  $V_{int2}$  is only suitable for the case of forward terminal voltage  $V$ . That is also identical to the results of  $V_{int}$  on the condition that  $V > 0$  V, as shown in Fig. 4. Of course, there is a transition region, where both  $I_R$

and  $I_E$  are not the dominant item in RHS of (3). Therefore, in this transition region, neither  $V_{int1}$  nor  $V_{int2}$  agree with  $V_{int}$  calculated through the Newton-Raphson root-finding scheme and the method of least squares from (3). However, by using smoothing function to choose the smaller value between  $V_{int1}$  and  $V_{int2}$ , and then, using Schroder series to improve the accuracy of computation results, we derive the explicit expression of  $V_{int}$  from (3) in this paper. It is noted that  $V_{int}$  calculated in (10) has a good match with the numerical iteration results of  $V_{int}$  in Fig. 4, especially for the transition region. In addition, Fig. 5 shows that the errors come into the scale of  $10^{-16}$  V.

Substituting (10) into (4), we can obtain the explicit calculation scheme of OSCs'  $I$ - $V$  characteristics. Furthermore, we show and compare the  $I$ - $V$  characteristics of OSCs simulated by equivalent circuits in Figs. 2 and 3. We can observe from Fig. 6 that the simulation results of

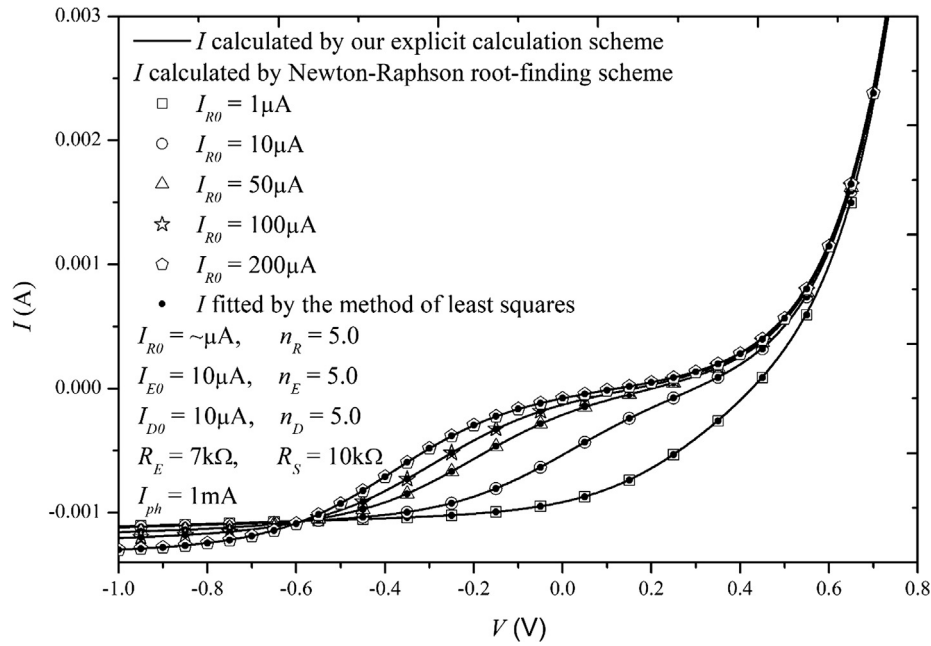


Fig. 12. Effects from  $I_{R0}$  on  $I$ - $V$  characteristics of OSCs simulated by our lumped-parameter circuits.

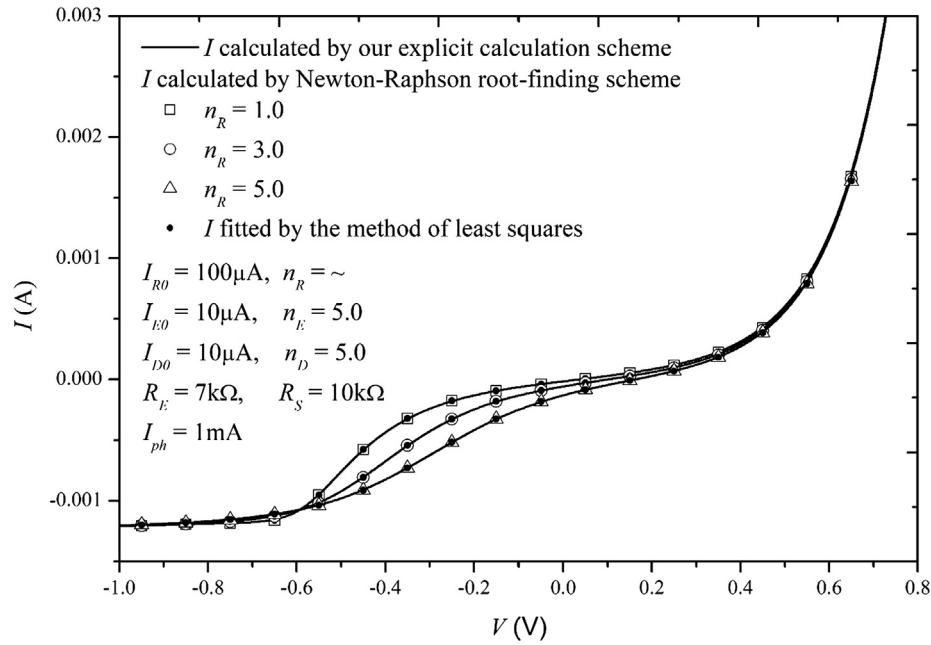


Fig. 13. Effects from  $n_R$  on  $I$ - $V$  characteristics of OSCs simulated by our lumped-parameter circuits.

OSCs'  $I$ - $V$  characteristics obtained from the lumped-parameter circuits in Figs. 2 and 3 are nearly consistent with each other. In other words, the circuits in Figs. 2 and 3 are equivalent. Of course, we also choose the simpler circuit in Fig. 2 instead of that in Fig. 3 to complete the simulations for the S-shaped  $I$ - $V$  characteristics of OSCs.

#### 4. Verification and discussion

##### A. Numerical iteration verification and discussion about fitting parameter effects

In this section, we use the method of least squares and Newton-Raphson root-finding scheme to fit and calculate the terminal current-voltage characteristics in Fig. 2, i.e., equation set of (3) and (4). And

then, we use our explicit calculation scheme presented in Part 3 to solve  $V_{int}$  from (3) and substitute  $V_{int}$  into (4) to obtain  $I$ - $V$  characteristics. Furthermore, we compare our results with numerical iteration results and discuss about the effects of the fitting parameters in Fig. 2 on the S-shaped  $I$ - $V$  characteristics of OSCs.

The current source  $I_{ph}$  in Fig. 2 describes the net polaron generation rate of OSCs under illumination. In the cases of the different illumination intensities,  $I_{ph}$  proportional to illumination intensity influent directly the  $I$ - $V$  characteristics in the third quadrant, as shown in Fig. 7. Obviously, the  $I$ - $V$  curves shift downward as illumination intensity increases. It is noted that the offsets of the  $I$ - $V$  curves in the third quadrant for  $I_{ph}$  result from the shunt resistance  $R_S$ . In Fig. 8,  $R_S$  determines the slope of the  $I$ - $V$  curve in the third quadrant and the terminal current magnitude of the  $I$ - $V$  curve in the first quadrant. On the one hand, the

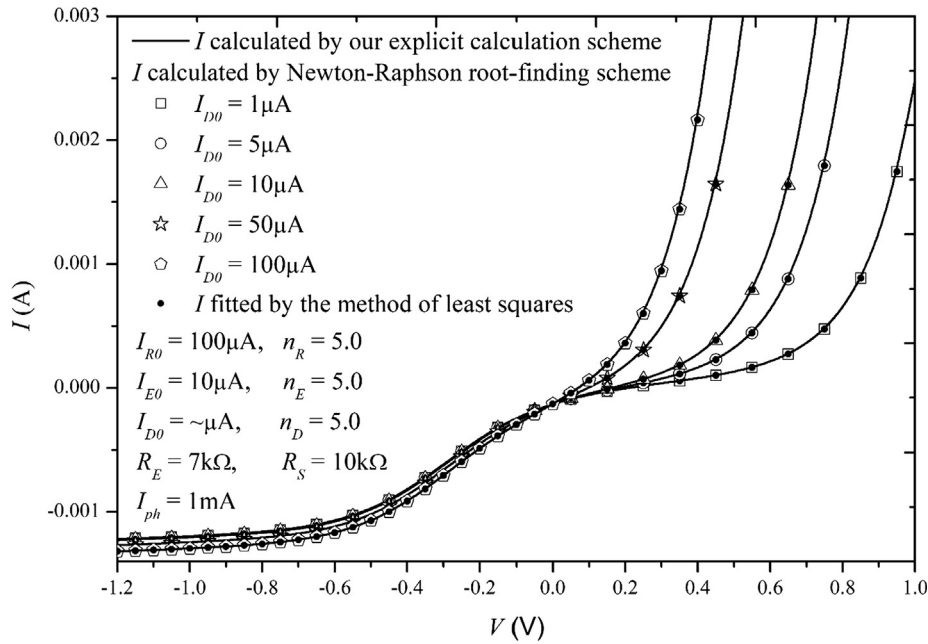


Fig. 14. Effects from  $I_{D0}$  on  $I$ - $V$  characteristics of OSCs simulated by our lumped-parameter circuits.

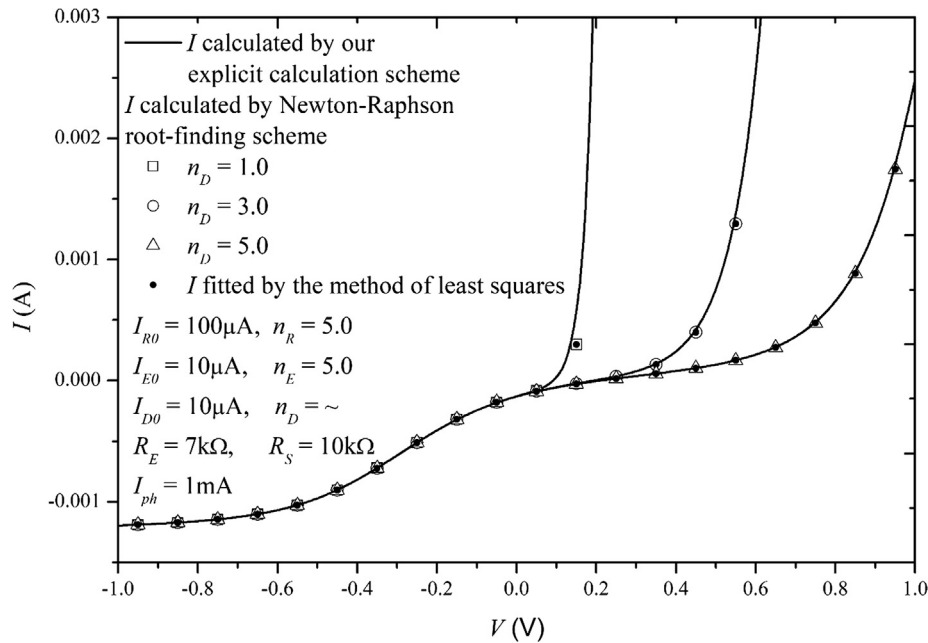


Fig. 15. Effects from  $n_D$  on  $I$ - $V$  characteristics of OSCs simulated by our lumped-parameter circuits.

slope of the  $I$ - $V$  curve decreases with the increment of  $R_S$  in the third quadrant. On the other hand, the terminal current magnitude of the  $I$ - $V$  curve also decreases with the increment of  $R_S$  in the third quadrant. In a word, we can observe from Fig. 8 that there is a negative correlation between the shunt resistance  $R_S$  and power-conversion efficiency (PCE). In fact,  $R_S$  represents contact resistance of OSCs resulting from the interfaces between electrode and acceptor, between acceptor and donor, and between donor and electrode.

Compared with Mazhari's model (Mazhari, 2006) and our previous work (Xu et al., 2018), the main difference of our lumped-parameter equivalent circuit model is that the diode  $D_E$  in connection with the parallel resistance  $R_E$  represents the extraction current  $I_E$ , i.e., the sum of  $I_{E1}$  and  $I_{E2}$  in Fig. 2. In Figs. 9–11, we show that the parameters  $I_{E0}$ ,  $n_E$ , and  $R_E$  have influences on the S-shaped  $I$ - $V$  characteristics of OSCs.

According to Figs. 9 and 10, both  $I_{E0}$  and  $n_E$  affect the  $I$ - $V$  characteristics in the third quadrant. Obviously, large  $I_{E0}$  and small  $n_E$  can make the S-shaped  $I$ - $V$  characteristics of OSCs approach into the J-shape, which would lead to higher PCE. Of course, that is consistent with the device physics. Both large  $I_{E0}$  and small  $n_E$  result in large extraction current, corresponding to large PCE. Compared with functions of  $I_{E0}$  and  $n_E$ ,  $R_E$  also play an important role in increasing the extraction current of OSCs with the decrease of  $R_E$ . As shown in Fig. 11, in the case of small  $R_E$ , the  $I$ - $V$  curve is J-shape leading to relative large PCE of OSCs. However, as  $R_E$  increases, the extraction current decreases. That would reduce the PCE of OSCs. As a result, the  $I$ - $V$  curve would deviate J-shape and transfer into S-shape, as shown in Fig. 11. It is noted that  $D_E$  only influence those in the third quadrant, and  $R_E$  can affect the  $I$ - $V$  curves in the first and third quadrants. In actual OSCs,  $I$ - $V$  characteristics in the first



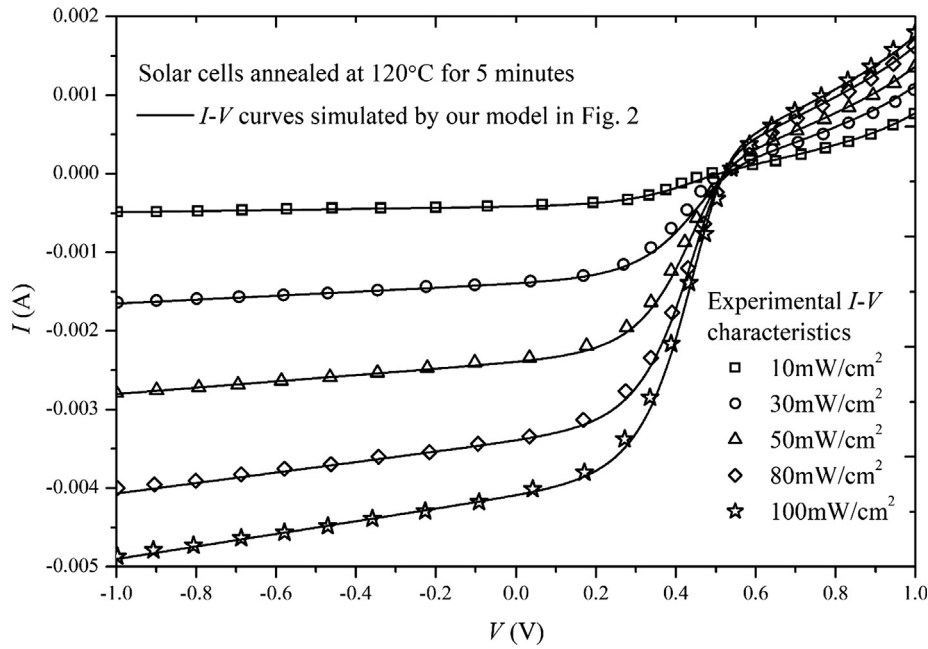


Fig. 16.  $I$ - $V$  characteristics of OSCs annealed at 120 °C for 5 min, simulated by our model and measured in (Laudani et al., 2018).

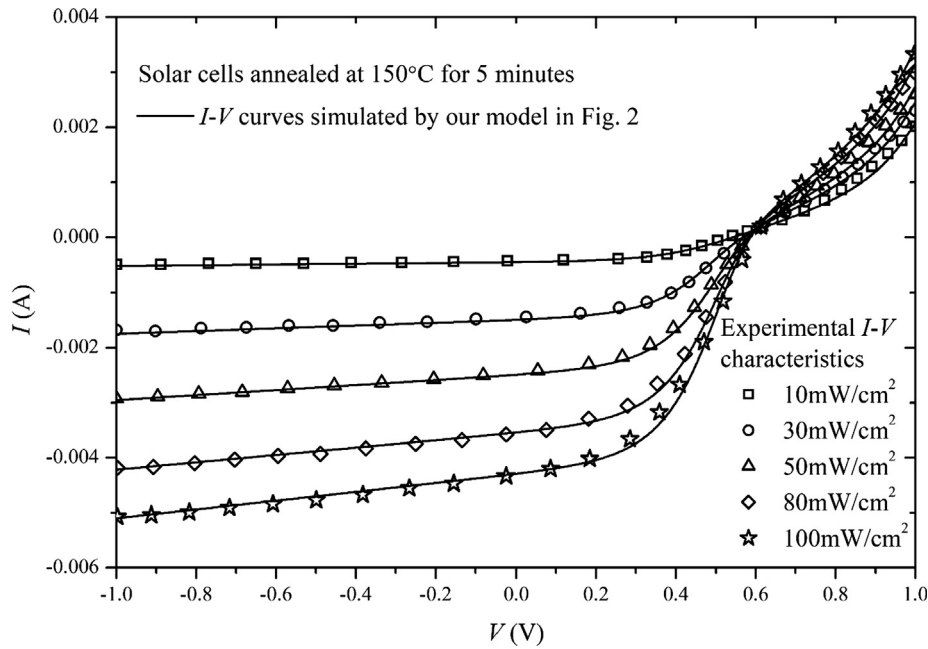


Fig. 17.  $I$ - $V$  characteristics of OSCs annealed at 150 °C for 5 min, simulated by our model and measured in (Laudani et al., 2018).

quadrant is exponent-like rise instead of exponent rise described by only one diode  $D_E$  Mazhari's model (Mazhari, 2006) and our previous model (Xu et al., 2018). In this paper, we use both the diode  $D_E$  and the shunt resistance  $R_E$  to demonstrate the extraction current. If  $R_E$  tends towards infinity, the lumped-parameter circuit degrades into Mazhari's model (Mazhari, 2006) and our previous model (Xu et al., 2018) so that the  $I$ - $V$  curves in the first quadrant approach to exponent rise. If  $R_E$  tends towards zero,  $I_{E2}$  would be much larger than  $I_{E1}$  in Fig. 2 so that the  $I$ - $V$  curves in the first quadrant approach to line rise.

The Diode  $D_R$  simulates the recombination current of OSCs and Figs. 12 and 13 show that the effects of  $I_{R0}$  and  $n_R$  on the  $I$ - $V$  characteristics. In contrast to the effects of  $D_E$ , the larger recombination current through  $D_R$  leads to low PCE of OSCs. In Figs. 12 and 13, for smaller  $I_{R0}$  and larger  $n_R$ , PCE is larger. The Diode  $D_D$  simulates the dark

current of OSCs and Figs. 14 and 15 show that the effects of  $I_{D0}$  and  $n_D$  on the  $I$ - $V$  characteristics. According to Figs. 14 and 15, large  $I_{D0}$  and small  $n_D$  can lead to large  $I_D$  corresponding with large PCE.

## B. Experiment verification

In Figs. 16–20, we compare the  $I$ - $V$  characteristics simulated by our proposed lumped-parameter circuit in Fig. 2 with the reconstructed experimental data (Laudani et al., 2018) of OSCs and obtain the good agreements on the different conditions of annealing temperature and illumination intensity. The fitting parameters used in simulations are listed in Table 1., that can be extracted through the common routine of the parameter acquisition (Mazhari, 2006). We make use of organic solar cells (Laudani et al., 2018), consisting of an enhanced bi-layer of

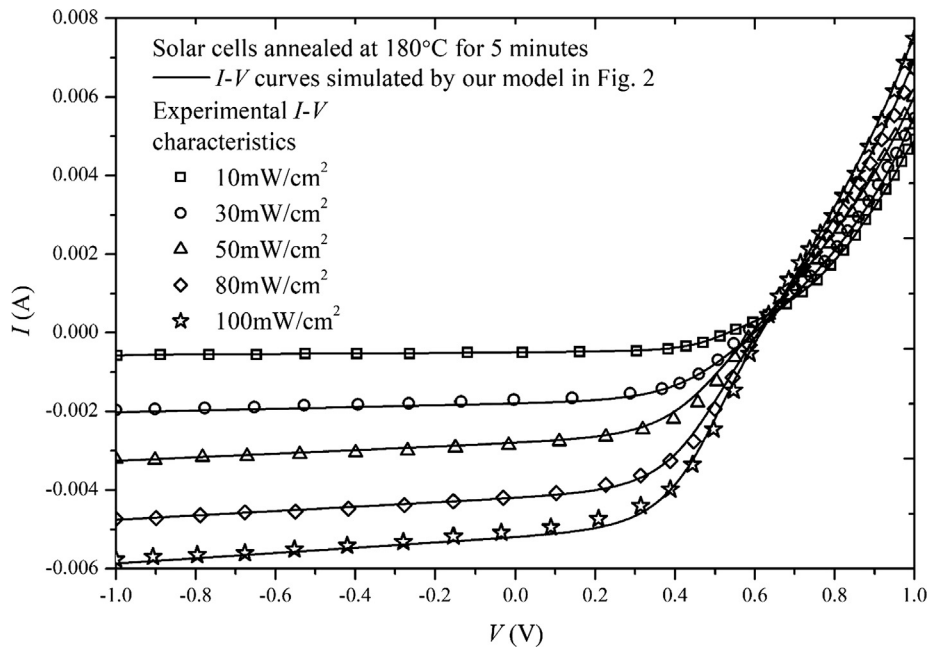


Fig. 18. *I-V* characteristics of OSCs annealed at 180 °C for 5 min, simulated by our model and measured in (Laudani et al., 2018).

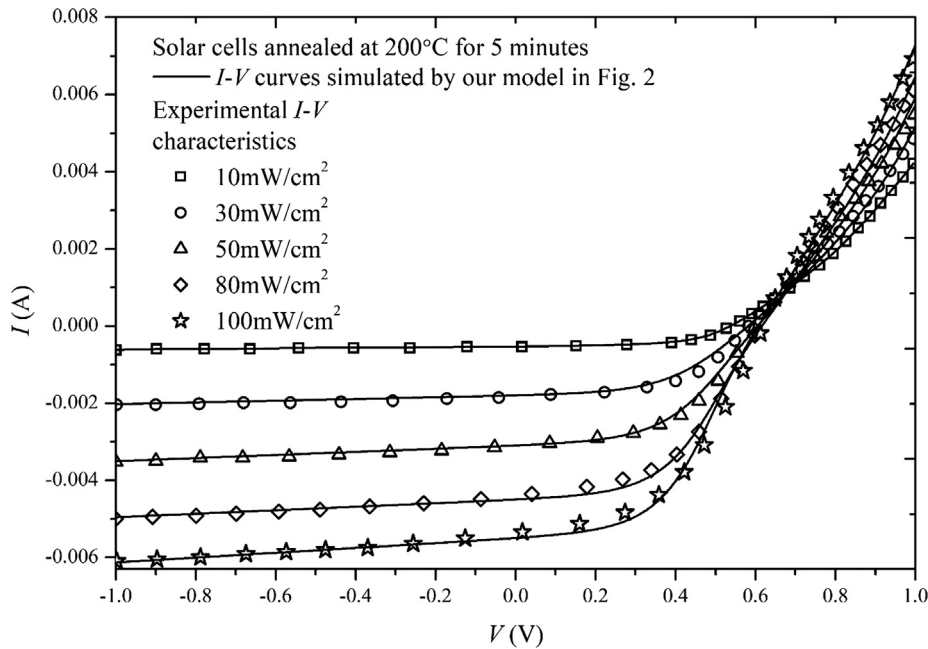


Fig. 19. *I-V* characteristics of OSCs annealed at 200 °C for 5 min, simulated by our model and measured in (Laudani et al., 2018).

purified Poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylene-vinylene] (MEH-PPV,  $M_n = 40,000$ – $70,000$ , Aldrich) acting as electron donor and fullerene C60 (> 99.95%, SES Research) acting as electron acceptor. Films were fabricated on cleaned ITO-coated glass coated with 50 nm of PEDOT:PSS (Aldrich, conductivity  $1 \text{ S cm}^{-1}$ ) and subsequently coated with 50 nm of Al to serve as the cathode.

Under the  $\text{N}_2$  atmosphere, the OSCs were exposed to the different illumination intensities (i.e.,  $10 \text{ mW/cm}^2$ ,  $30 \text{ mW/cm}^2$ ,  $50 \text{ mW/cm}^2$ ,  $80 \text{ mW/cm}^2$ ,  $100 \text{ mW/cm}^2$ ) simulated AM1.5G sunlight, and the *I-V* characteristics were measured and shown as symbols in Figs. 16–19. It is noted that larger illumination intensity in measurement needs larger  $I_{ph}$  in our model to complete simulating the *I-V* characteristics of OSCs. In addition, we can observe from Fig. 20 that higher thermal annealing temperature can be used to reduce the S-shape, leading to higher PCE of

OSCs.

## 5. Conclusions

In this paper, we proposed an improved lumped-parameter equivalent circuit model of organic solar cells to give the accurate descriptions about the S-shaped *I-V* characteristics. Firstly, we present the circuit structure of the lumped-parameter model and its equivalent circuit following Miller theorem. Secondly, we derive the explicit expression of the *I-V* characteristics based on the regional approach. Thirdly, we verify the simulation results of our model by using Newton-Raphson root-finding scheme and the method of least squares and discuss about effects from fitting parameters on the *I-V* curves of OSCs. Finally, we compare simulation results with reconstructed experimental

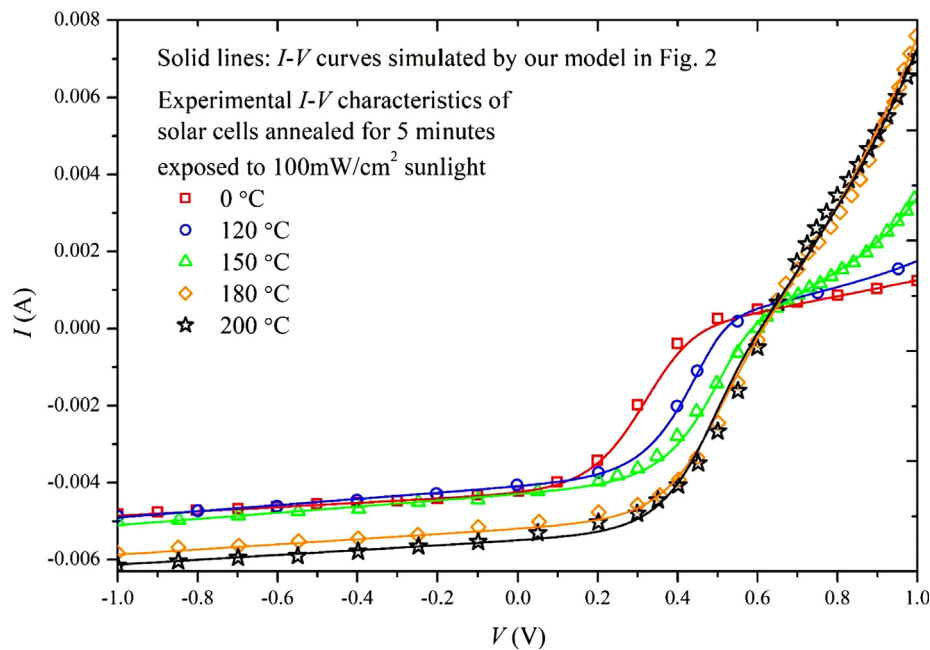


Fig. 20. *I-V* characteristics of OSCs annealed different temperatures, simulated by our model and measured in (Laudani et al., 2018).

Table 1

Parameters for simulations of our model.

Symbol (units)	No annealing	Annealing at 120 °C	Annealing at 150 °C	Annealing at 180 °C	Annealing at 200 °C
Illumination (mW/cm <sup>2</sup> )	–	10,30,50,80,100	10,30,50,80,100	10,30,50,80,100	10,30,50,80,100
$I_{RO}$ (μA)	2.5	2.5	2.0	2.0	2.0
$I_{EO}$ (μA)	30	30	30	30	30
$I_{DO}$ (nA)	0.012	12	15	15	15
$n_R$	2.9	4, 3.5, 3.2, 3.1, 3.0	4, 3.5, 3.4, 3.3, 3.2	4, 3.5, 3.3, 3.2, 3.1	4, 3.4, 3.3, 3.1, 3.0
$n_E$	1.8	1.0	1.0	1.0	1.0
$n_D$	6.2	4.0	3.5	3.5	3.5
$R_E$ (kΩ)	0.65	0.8,0.6,0.55,0.55,0.55	0.3,0.3,0.26,0.22,0.20	0.08,0.07,0.07,0.06,0.05	0.08,0.07,0.06,0.06,0.05
$R_S$ (kΩ)	1.8	15, 4, 2.5, 1.5, 1.25	15, 4, 2.2, 1.5, 1.25	10, 4.5, 2.2, 1.8, 1.5	10, 4.5, 2.5, 2.2, 1.6
$I_{ph}$ (mA)	4.3	0.42, 1.4, 1.6, 3.4, 4.1	0.45, 1.5, 2.5, 3.5, 4.3	0.5, 1.8, 2.8, 4.2, 5.2	0.5, 1.8, 3.5, 4.5, 5.5

data to valid our model. As a result, such a model can be adopted as the useful platform to electrically explain the S-shaped *I-V* characteristics of OSCs and complete computer-aided-design system of photovoltaic applications.

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