Exact analytical solution for organic solar cells showing S-shaped J-V characteristics using Special Trans Function Theory (STFT)

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Received: 22.05.2013 Accepted: 15.06.2013

Abstract- Many organic solar cells exhibit anomalous kinks showing S-shaped J-V behaviour. This atypical behaviour may be electrically modelled by including a second diode (D_2) with opposite current characteristics together with a shunt resistance to that of the conventional solar cell diode (D_1). In this communication, we present an exact analytical expression for the cell's output voltage as an explicit function of its terminal current by the application of special trans function theory (STFT) for the S-shaped J-V characteristics model. The explicit nature of the proposed solution avoids approximations and numerical iterations. The differentiability of the trans function in STFT facilitates the analytical analysis of the problem. The evolution of the S-shaped J-V characteristics and the fill factor (FF) is also deliberated by varying different parameters to validate the proposed analytical solution.

Keywords- Organic Solar Cells (OSC), S-shaped kinks, Solar Cell Model, STFT.

1. Introduction

The development of organic solar cells (OSCs) has quickly progressed in the last few years making it as the potential alternative to conventional inorganic photovoltaic devices. They have certain latent advantages such as: low-cost and ease of processing, amalgamation onto unconventional substrates, and the existence of a vast variety of organic structures whose functionalities can be chemically tuned to adjust the energy levels thereby improving light absorptions and charge transport. Currently, power conversion efficiency has reached as high as 8 to 9% [1]. Even so, OSCs have yet to achieve conversion efficiencies that would make them competitive. Consequently, substantive basic research and development is still going on in OSC materials, structures, and processing techniques. The analysis of the cells' current density-voltage (J-V) characteristics is one of the essential tools for this task [2].

Many of the developmental OSCs exhibit anomalous S-shaped "kinks" in their J-V characteristics [3-9], which are attributed to (i) the local space charges in multilayer devices [5], (ii) the contact and other interface phenomena [6-8] and (iii) the strong imbalance of charge carrier mobilities in the photoactive material [9]. This atypical behavior results in a significant reduction in the fill factor and the overall conversion efficiency of the cell, whence it is detrimental to the device parameters. The standard equivalent circuit of solar cells based on the single diode model having parasitic resistances cannot explain this anomalous behavior. On the other hand, electrical modeling enables quantitative analysis of its emergence and evolution. In particular, a modified form of the conventional single-diode solar cell equivalent circuit was proposed to account for the anomalous S-shaped "kink" observed in many OSC devices [6].

Analytical solutions are always welcome especially in solving the transcendental J-V equations of solar cells. One crucial method of solving the J-V transcendental equation based on the single-diode circuit model is the use of special trans function theory (STFT) [12], which have been used to investigate various parameters of real solar cells [13-15]. Solving the modified two-diode circuit model [6] leads to a system of transcendental equations which, to our knowledge, has been solved using approximations [6] and numerical methods [10] as well as by the method of Lambert W-function [11]. This communication presents, an exact analytical solution for this model using STFT. The general applicability of STFT for arbitrary nonlinear forms [12] enables to solve the system of transcendental equations to obtain an explicit expression for the terminal voltage in terms of the current density and other circuital parameters. This technique reduces the computation time to simulate and fit the J-V curves. Also, the influence of the new circuital component on the entire S-shape is carried out by varying the associated parameter.

2. Theory

Fig. 1 shows the proposed modified equivalent circuit model [6] to account the appearance of anomalous kink in the J-V characteristics of OSCs. It incorporates a series-connected additional circuit (III), consisting of a parallel combination of a reverse-connected diode (D_2) and a shunt resistance with the conventional single-diode equivalent circuit of a solar cell (consisting of sub-circuits (I) & (II). When no current flows through the counter diode (J_{d2}=0), the circuit is reduced to the conventional equivalent circuit with the series resistance given by $R_s + R_{P2}$.

The terminal voltage is given by the sum of the voltages of three series-connected subparts (namely (I), (II) and (III)

$$V = V_R + V_{d1} + V_{d2} = JR_s + J_{RP1}R_{P1} + J_{RP2}R_{P2} \tag{1}$$

where V_{d1} and V_{d2} are the voltage drops across parallel resistances R_{P1} and R_{P2} respectively, and J_{RP1} and J_{RP2} are the currents flowing through them.

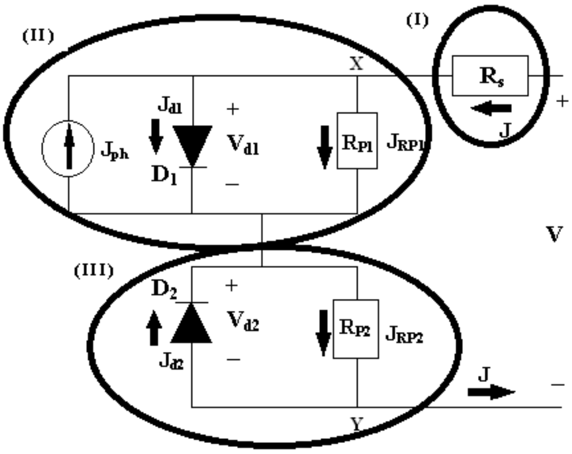

Fig. 1. Equivalent circuit including a second diode (D_2) with opposite current characteristics to that of the conventional solar cell diode (D_1) for OSC showing S-shaped J-V characteristics

Application of Kirchoff's current law at X and Y leads to equations (2) and (3) respectively:

$$J_{RP1} = J + J_{ph} - J_{d1} \tag{2}$$

$$J_{RP2} = J + J_{d2} \tag{3}$$

where J_{d1} and J_{d2} are the currents through diodes D_1 and D_2 respectively, which are given by

$$J_{d1} = J_{01}\left(e^{\frac{V_{d1}}{n_1 v_{th}}} - 1\right) \tag{4}$$

$$J_{d2} = J_{02}\left(e^{\frac{-V_{d2}}{n_2 v_{th}}} - 1\right) \tag{5}$$

Now the terminal current flowing through the series-connected subparts (namely (I), (II) and (III) in Fig. 1) can be represented by one of the following three equations:

$$J = \frac{V_R}{R_s} \tag{6}$$

$$J = J_{01}\left(e^{\frac{V_{d1}}{n_1 v_{th}}} - 1\right) + \frac{V_{d1}}{R_{P1}} - J_{ph} \tag{7}$$

$$J = -J_{02}\left(e^{\frac{-V_{d2}}{n_2 v_{th}}} - 1\right) + \frac{V_{d2}}{R_{P2}} \tag{8}$$

where J_{01} and J_{02} are the reverse saturation currents, n_1 and n_2 are the ideality factors for diodes D_1 and D_2 respectively, v_{th} (=K_BT/q) is the thermal voltage and J_{ph} is the photogenerated current.

The explicit form of the terminal voltage may be obtained by explicitly solving for V_{d1} and V_{d2} from (7) and (8) respectively. This is accomplished by the application of STFT [12-15], an analytical technique especially used for solving transcendental equations.

With some mathematical rearrangements, Eq. (7) may be rewritten as

$$\left[\frac{R_{P1}\left(J + J_{ph} + J_{01}\right) - V_{d1}}{n_1 v_{th}}\right] = \frac{J_{01}R_{P1}}{n_1 v_{th}} e^{\frac{R_{P1}\left(J + J_{ph} + J_{01}\right)}{n_1 v_{th}}} e^{-\left[\frac{R_{P1}\left(J + J_{ph} + J_{01}\right) - V_{d1}}{n_1 v_{th}}\right]} \tag{9}$$

reducing to the transcendental form of

$$\psi_1(\zeta) = U_1(\zeta)e^{-\psi_1(\zeta)}, U_1(\zeta) \subset R^+ \tag{10}$$

The solution, according to STFT is

$$\psi_1(\zeta) = trans_+\left(U_1(\zeta)\right) \tag{11}$$

Here $trans_+(U_1(\zeta))$ is a new special trans function [12-15] defined as

$$trans_+\left(U_1(\zeta)\right) = \lim_{x\to\infty}\left[\ln\left(\frac{\varphi\left(x+1, U_1(\zeta)\right)}{\varphi\left(x, U_1(\zeta)\right)}\right)\right] \tag{12}$$

with

$$\varphi\left(U_1(\zeta)\right)=\sum_{m=0}^{[x]}\frac{\left(U_1(\zeta)\right)^m (x-m)^m}{m!} \tag{13}$$

where

$$\psi_1(\zeta)=\frac{R_{P1}\left(J+J_{ph}+J_{01}\right)-V_{d1}}{n_1 v_{th}} \tag{14}$$

and

$$U_1(\zeta)=\frac{J_{01}R_{P1}}{n_1 v_{th}}e^{\frac{R_{P1}\left(J+J_{ph}+J_{01}\right)}{n_1 v_{th}}} \tag{15}$$

Using Eqs. (11) & (14), the explicit expression of Vd1 can be written as

$$V_{d1}=\left(J+J_{01}+J_{ph}\right)R_{P1}-n_1 v_{th}\left(trans_+ U_1(\zeta)\right) \tag{16}$$

Similarly, Eq. (8) can be rewritten as

$$\left[\frac{V_{d2}-R_{P2}\left(J-J_{02}\right)}{n_2 v_{th}}\right]=\frac{J_{02}R_{P2}}{n_2 v_{th}}e^{\frac{-R_{P2}\left(J-J_{02}\right)}{n_2 v_{th}}}e^{-\left[\frac{V_{d2}-R_{P2}\left(J-J_{02}\right)}{n_2 v_{th}}\right]} \tag{17}$$

This is of the transcendental form of

$$\psi_2(\zeta)=U_2(\zeta)e^{-\psi_2(\zeta)},U_2(\zeta)\subset R^+ \tag{18}$$

whose solution according to STFT is

$$\psi_2(\zeta)=trans_+\left(U_2(\zeta)\right) \tag{19}$$

Here $trans_+(U_1(\zeta))$ is the new special trans function [12-15] defined as

$$trans_+\left(U_2(\zeta)\right)=\lim_{x\to\infty}\left[\ln\left(\frac{\varphi\left(x+1,U_2(\zeta)\right)}{\varphi\left(x,U_2(\zeta)\right)}\right)\right] \tag{20}$$

with

$$\varphi\left(U_2(\zeta)\right)=\sum_{m=0}^{[x]}\frac{\left(U_2(\zeta)\right)^m (x-m)^m}{m!} \tag{21}$$

where

$$\psi_2(\zeta)=\frac{V_{d2}-R_{P2}\left(J-J_{02}\right)}{n_2 v_{th}} \tag{22}$$

and

$$U_2(\zeta)=\frac{J_{02}R_{P2}}{n_2 v_{th}}e^{\frac{-R_{P2}\left(J-J_{02}\right)}{n_2 v_{th}}} \tag{23}$$

From Eqs. (19) & (22), we obtain the expression for Vd2 as

$$V_{d2}=\left(J-J_{02}\right)R_{P2}+n_2 v_{th}\left(trans_+ U_2(\zeta)\right) \tag{24}$$

Substitution of Eqs. (16) and (24) into (1) yields the analytical expression of the terminal voltage in terms of current and the circuital parameters

$$V=JR_s+\left(J+J_{01}+J_{ph}\right)R_{P1}-n_1 v_{th}\left(trans_+ U_1(\zeta)\right)+\left(J-J_{02}\right)R_{P2}+n_2 v_{th}\left(trans_+ U_2(\zeta)\right) \tag{25}$$

3. Results and Discussion

The scope of this communication is to obtain an explicit analytical expression to model the J-V curves showing S-shape observed in many organic solar cells, for the proposed electrical model [6]. Nevertheless, it is not feasible to express the terminal current as an explicit function of the terminal voltage. Notwithstanding this, Eq. (25) is still very useful as it involves no approximations or iterative numerical procedures.

In order to validate the analytical expression of Eq. (25) obtained by STFT, we simulate the J-V curve showing S-shape using the following parameters: R_{P1} = 10 kΩ , R_{P2} = 1.2 kΩ , R_s = 0.0 Ω, J_{01} = 0.14 mA/cm^2, J_{02} = 0.4 mA/cm^2 , J_{ph} = 1.1 mA/cm^2, n_1 = 6.5, n_2 = 3.0. These parameter values are comparable to the recently extracted data of OSCs [10]. In Fig. 2, current densities J, J_{d1} and J_{d2} are plotted against voltage in order to compare them. It also shows the effect of changing R_{P1} on the total S-shaped J-V characteristics of an OSC. It is seen that on decreasing R_{P1}, the short-circuit current as well as the open-circuit voltage of the illuminated J-V characteristics reduces.

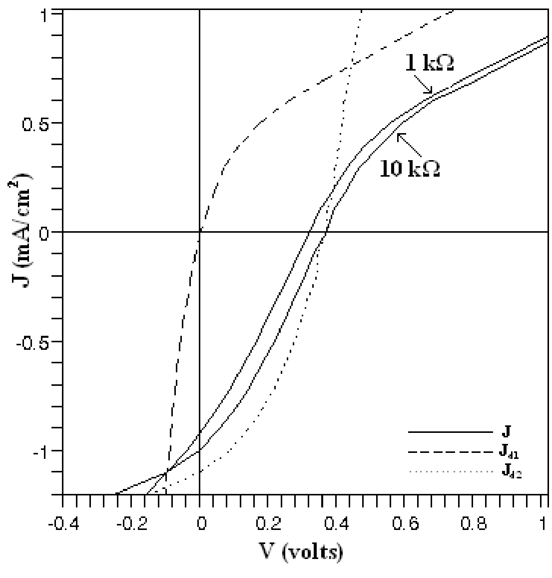

Fig. 2. J-V characteristic curve of a hypothetical organic solar cell showing S-shape using the analytical expression of Eq. (25) for two different values of R_{01} using STFT.

Further, this solution is also used to analyze the effect of the various model parameters, especially that of diode (D_2), on the cell's J-V characteristics. To see these impacts, various J-V curves have been simulated for different values of J_{02} and R_{P2} by keeping the remaining parameters at the same values as in Fig. 2 so as to ensure the S-shape in the J-V curve. Fig. 3 illustrates the effect of J_{02} on the evolution of the S-shape J-V curve. It is observed that the value of J_{02} determines the position of the convexity in the S-shape curve.

Similarly, Fig. 4 depicts the evolution of the J-V curve for different values of R_{P2}. It is worth mentioning that when R_{P2} decreases, the total current through it increases and the kink in the J-V curve disappears. It is seen that, by choosing a proper parameter value of J_{02} and R_{P2}, we have a wide range of possible combinations to describe the appearance of S-shape in the J-V characteristics of OSCs.

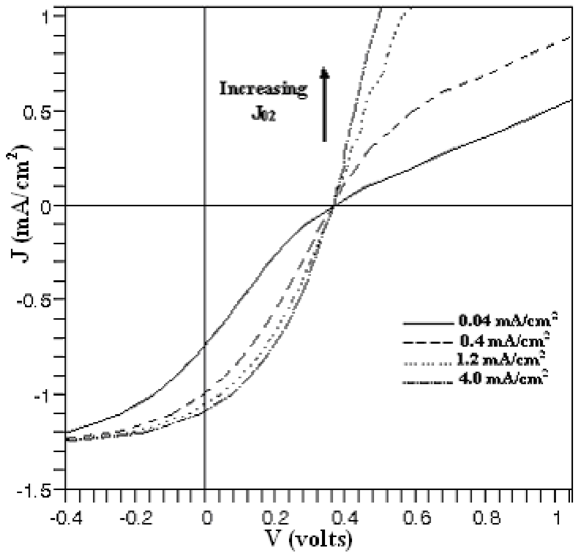

Fig. 3. Effect of J_{02} on the S-shape J-V curve of a hypothetical organic solar cell using the analytical expression of Eq. (25) using STFT.

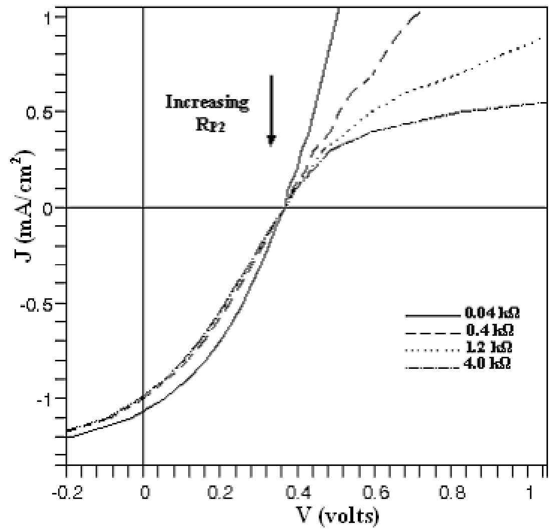

Fig. 4. Effect of R_{02} on the S-shape J-V curve of a hypothetical organic solar cell using the analytical expression of Eq. (25) using STFT.

On the other hand, the existence of different gradients in STFT [8] makes it possible to perform an analytical analysis of any physical process. Consequently, Eq. (25) may be analytically differentiated with respect to its internal parameters, whence various parameters can be determined. For example, the evolution of the fill factor (FF) for a pristine device showing S-shape J-V curve [10] with R_{P2} and J_{02} is shown in Fig. 5 and Fig. 6 respectively. The parameters for this pristine device are: J_{01}=0.14 mA/cm^2, J_{02}=0.42 mA/cm^2, R_{P1}=0.66 MΩ, R_{P2}=6.4 kΩ, n_1=6.5, n_2=3.0, T=300 K.

It is observed that FF decreases as R_{P2} increases (Fig. 5). Moreover, it is also seen that the variation of FF with J_{02} shows a minima which is expected for any J-V curve exhibiting an S-shape (Fig. 6). These observations are in accordance with the conclusions of [11].

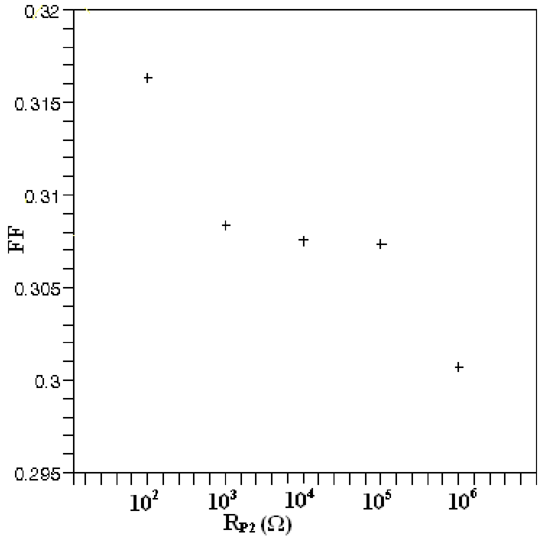

Fig. 5. Evolution of the fill factor (FF) of a pristine solar cell for different values of R_{P2}

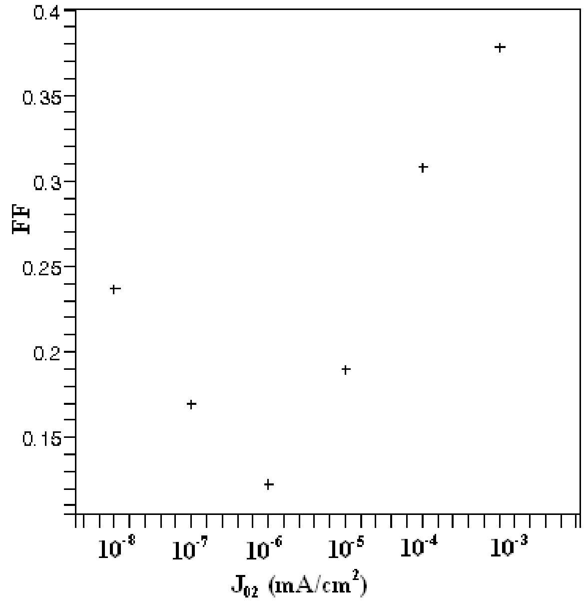

Fig. 6. Evolution of the fill factor (FF) of a pristine solar cell for different values of J_{02}

4. Conclusion

We have presented, by the application of STFT, an explicit form of the terminal voltage in terms of the terminal current and the model's parameters of OSCs showing S-shape in its

J-V characteristics from the equivalent circuit that reproduces the kink. This expression optimizes the calculations and the parameter extraction. The explicit nature also facilitates the analytic differentiation because of the existence of gradients in STFT. The evolution of the J-V curve and FF for different values of J_{02} and R_{P2} is studied in order to perceive the role of the additional sub-circuit (III) which is in agreement to the reported results. This validates the proposed analytical method of STFT in the study of organic solar cells through its explicit solutions according to the proposed electrical model.

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