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Exact analytical solution of a two diode circuit model for organic solar cells showing S-shape using Lambert W-functions

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Abstract

Organic solar cells (OSCs) often show a kink, also called S-shape, in the current–voltage (I–V) characteristics, that has been attributed to different physical phenomena such as poor quality of cathode-active layer interface or unbalance charge carrier mobilities. This non-ideal behaviour can be electrically modelled including a second diode, in reverse bias, together with an extra shunt resistance (R_{P2}) in the traditional solar cell equivalent circuit. In this paper, we solve without approximations the transcendental equation system derived from this modified circuit. We have obtained an analytical expression for I–V curves decoupling the voltage drop in each diode using Lambert W function. This expression has been fitted to experimental data in order to obtain circuital parameters. Simulations varying saturation current of reverse diode (I_{02}) and R_{P2} have been performed in order to study the dependence of S-shape with these parameters.
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1. Introduction

Organic solar cells development has quickly progressed during the last years due to their possibilities to be fabricated onto light, thin and flexible substrates with a low cost processing technology (Brabec et al., 2001). Currently, power conversion efficiency (PCE) has reached values around 8% for polymer:fullerene based devices (Chen et al., 2009). However, PCE and fill factor (FF) are dramatically affected when I–V characteristic exhibits a kink shape in the fourth quadrant. Many authors have observed this effect in different materials and structures (Lilliedal et al., 2010; Glatthaara et al., 2007; Vogel et al., 2006) and have attributed it to different causes such as a poor quality of polymer–cathode interface (Gupta et al., 2008; Castro et al., 2010), the presence of strong interface dipoles (Kumar et al., 2009), or to the strong unbalance of charge carrier mobilities in the photoactive material (Tress et al., 2011). This atypical behaviour cannot be electrical modelled with the standard equivalent circuit of solar cells consisting on an ideal diode in parallel with a current source, shunt resistance and series resistance (Wolf and Rauschenbach, 1963). A modified equivalent circuit, including an extra diode in reverse bias, together with its parallel resistance, was recently proposed to model the kink in these S-shape devices. Solution to this circuit has been obtained adopting approximations that may not be valid in the whole voltage range (Castro et al., 2010).

On the other hand, even in the case of the one-diode circuit model, obtaining an analytical solution is not an easy task and requires the use of tabulated Lambert W-function. This solution was first given for a circuit containing just a single diode with series resistance (Banwell, 2000), and then generalised for solar cells including photogenerated current and parallel resistance (Jain and Kapoor, 2004).

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When solving the two diode circuit model, it leads to a transcendental equation system that, to our knowledge, has only been solved doing some approximations (Castro et al., 2010) or by numerical methods (del Pozo et al., 2012). In this letter we present for the first time an exact analytical solution for this two diode circuit based on the Lambert W-functions. This analytical expression will reduce the computation time to simulate and fit *I–V* curves simplifying the parameter extraction. Moreover, the influence on the S-shape of the new circuital components is studied varying the corresponding parameters.

2. Model

Fig. 1 shows the modified equivalent circuit proposed by Castro et al. (2010) for modelling the kink in organic solar cells. An additional diode (*d*2) and its parallel resistance (R_{P2}) have been included in series with the standard circuit.

From the figure, applying Kirchoff's voltage law (KVL) the following expression relating V and I can be derived:

$$V = IR_S + V_1 + V_2 \tag{1}$$

Applying Kirchoff's current law (KCL) to node A and B leads to Eqs. (2) and (3) respectively:

$$I = I_{d1} + I_{RP1} - I_{PH} \tag{2}$$

$$I = I_{RP2} - I_{d2} \tag{3}$$

On the other hand, V_1 and V_2 are related to I_{d1} and I_{d2} as:

$$I_{d1} = I_{01}\left[\exp\left(\frac{V_1}{n_1KT}\right) - 1\right] \tag{4}$$

$$I_{d2} = I_{02}\left[\exp\left(\frac{-V_2}{n_2KT}\right) - 1\right] \tag{5}$$

where I_{01} and I_{02} are saturation currents and n_1 and n_2 are the ideality factors for diode1 and diode2 respectively. In order to generalise the expression, diodes parameters have been considered different.

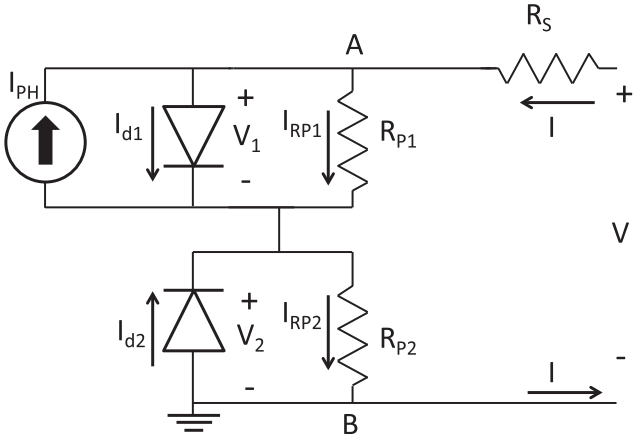

Fig. 1. Modified equivalent circuit including a new element (diode 2) opposite to the solar cell diode (diode 1).

Substituting Eq. (4) in Eqs. (2) and (5) in (3), and applying Ohm's Law to R_{P1} and R_{P2}, yields to the following equations:

$$I = I_{01}\left[\exp\left(\frac{V_1}{n_1KT}\right) - 1\right] + \frac{V_1}{R_{P1}} - I_{PH} \tag{6}$$

$$I = -I_{02}\left[\exp\left(\frac{-V_2}{n_2KT}\right) - 1\right] + \frac{V_2}{R_{P2}} \tag{7}$$

With these mathematical manipulations we have decoupled variables V_1 and V_2 in two separate equations. These expressions can be independently solved for V_1 and V_2 using Lambert W-function,

$$V_1 = (I + I_{PH} + I_{01})R_{P1} - \frac{n_1KT}{q}W\left\{\frac{q}{n_1KT}I_{01}R_{P1}\exp\left[\frac{q}{n_1KT}R_{P1}(I + I_{PH} + I_{01})\right]\right\} \tag{8}$$

$$V_2 = (I - I_{02})R_{P2} + \frac{n_2KT}{q}W\left\{\frac{q}{n_2KT}I_{02}R_{P2}\exp\left[\frac{-q}{n_2KT}R_{P2}(I - I_{02})\right]\right\} \tag{9}$$

Substituting Eqs. (8) and (9) in (1), voltage can be expressed analytically in terms of current and circuital parameters as:

$$V = (I + I_{PH} + I_{01})R_{P1} - \frac{n_1KT}{q}W\left\{\frac{q}{n_1KT}I_{01}R_{P1}\exp\left[\frac{q}{n_1KT}R_{P1}(I + I_{PH} + I_{01})\right]\right\} + \frac{n_2KT}{q}W\left\{\frac{q}{n_2KT}I_{02}R_{P2}\exp\left[\frac{-q}{n_2KT}R_{P2}(I - I_{02})\right]\right\} + (I - I_{02})R_{P2} + IR_S \tag{10}$$

3. Results and discussion

In order to validate the model, a new bunch of organic solar cells with structure ITO/PEDOT:PSS/P3HT:PCBM/Al were fabricated and characterised following experimental details given in del Pozo et al. (2012). Device active area is 7 mm^2. S-shape in *I–V* curves was achieved playing with the evaporation vacuum levels in order to obtain a bad quality polymer–cathode interface. Nevertheless, studying the physical causes responsible for this behaviour is beyond the scope of this work. Eq. (10) was fitted to experimental *I–V* curve in order to obtain electrical parameters. R_S was set to zero, as it was found in a previous work that this parameter was not necessary when fitting *I–V* curves in the low voltage region (del Pozo et al., 2012). The best fit parameters obtained were $I_{01} = 1.5 \times 10^{-5}$ A, $n_1 = 9.5$, $R_{P1} = 1.0 \times 10^{8}\ \Omega$, $I_{02} = 2.4 \times 10^{-7}$ A, $n_2 = 2.4$, $R_{P2} = 4.6 \times 10^{4}\ \Omega$ and $I_{PH} = 4.85 \times 10^{-5}$ A. As expected from devices showing S-shape, they do not show a good

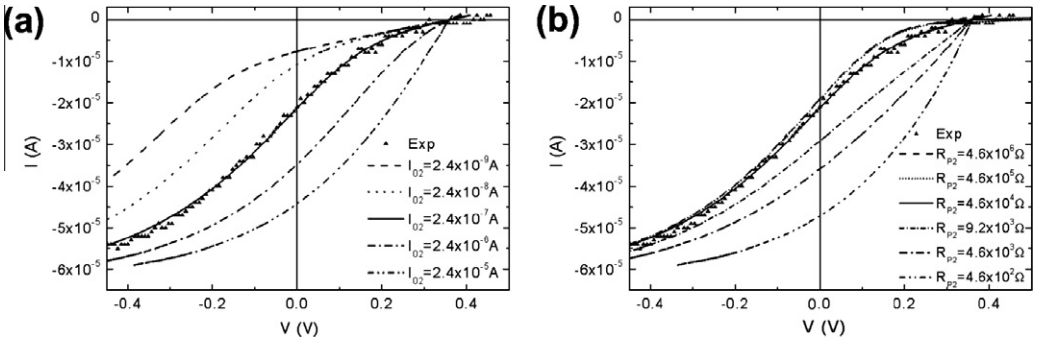

Fig. 2. (a) Experimental (symbols) and simulated I–V curves for different values of I_{02}, ranking from 2.4×10^{-9} A to 2.4×10^{-5} A. (b) Experimental (symbols) and simulated I–V curves for different values of R_{P2}, ranking from 460 Ω to 4.6 MΩ.

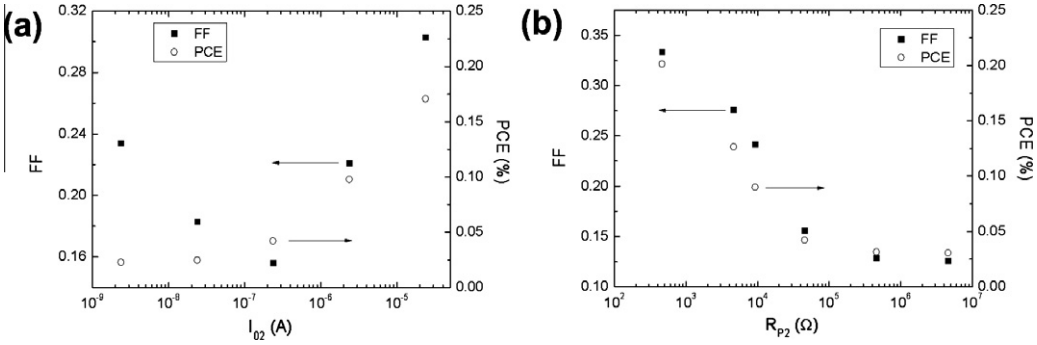

Fig. 3. (a) Evolution of FF and PCE with I_{02}. (b) Evolution of FF and PCE with R_{P2}.

performance and thus I_{PH} has a low value compared to a proper fabricated device.

It is worth mentioning that these rather high values for the ideality factor are often encountered in organic devices (Nehaoua et al., 2010; Shen et al., 2011). In order to study the evolution of the S-shape, simulations varying I_{02} and R_{P2} around this fitting values have been performed.

Fig. 2 shows the experimental data and theoretical I–V curves varying I_{02} from 2.4×10^{-9} A to 2.4×10^{-5} A (Fig. 2a) and R_{P2} from 460 Ω to 4.6 MΩ (Fig. 2b). Fig. 3 shows the evolution of FF and PCE with I_{02} and R_{P2}. As can be observed in Fig. 3a, PCE increases with I_{02}. On the other hand, FF shows a minimum around the value obtained in the fit as can be expected for an I–V curve exhibiting S-shape. Fig. 3b shows that an increase in R_{P2} results in a decrease of both FF and PCE.

It is worth noticing that when R_{P2} is very low, compared to diode 2 dynamical resistance, most of the current flows through R_{P2}, being the current flow through diode 2 negligible. In that case, the modified circuit becomes the traditional one, with total series resistance $R_{Stotal} = R_S + R_{P2}$. On the other hand, when I_{02} is very low, dynamic resistance of diode 2 is very high, resembling an open circuit. In this case modified circuit of Fig. 1 again becomes the one diode circuit with $R_{Stotal} = R_S + R_{P2}$. However if I_{02} is very high, dynamic resistance of diode 2 is very low, resembling a short circuit and bypassing R_{P2}. The modified circuit becomes once more the original one with $R_{Stotal} = R_S$. Only in the intermediate case, when diode 2 has a dynamic resistance similar to R_{P2} the kink appears.

4. Conclusions

For the first time, an exact explicit analytical solution for I–V characteristics of OSC showing S-shape based on Lambert W function is given. The role of the second extra diode and of its parallel resistance has been studied simulating I–V curves varying these parameters. Simulations show that S-shape disappears when R_{P2} decreases and when I_{02} increases. Electric parameters have been obtained fitting the model to experimental data.

Acknowledgements

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