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An in-depth analysis of the modelling of organic solar cells using multiple-diode circuits

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ABSTRACT

In this paper, an in-depth analysis of the current–voltage characteristics of organic solar cells is performed by introducing a new one-equation model based on a generalised equivalent circuit capable of accurately fitting ideal and non-ideal curves. The model is based on the introduction of a non-linear series resistance term that can be reduced to a linear resistance for the case of ideal curves. A hybrid optimiser approach is proposed combining genetic algorithms and deterministic methods that is shown to facilitate the extraction of the parameters and to accelerate the analysis of the identification problem. Our model is compared with state-of-the-art circuits found in the literature and validated though successful fitting of several experimental curves with differing levels of non-ideal behaviour (such as kinks and s-shape).

1. Introduction

Organic solar cells (Organic PhotoVoltaic – OPV) are approaching commercial viability with reported power conversion efficiency of over 13% and encouraging lifetimes (Green et al., 2016; Kong et al., 2014; Heliatek, 2016). Different from crystalline silicon (c-Si) cells, OPVs are not a single technology as manufacturers and research labs use different active layer materials (e.g. organic semiconductor, interlayers, etc.) and various device architectures. That poses challenges to development of the area. One way to accelerate the optimisation and identification of issues during R&D and upscaling is through the development of a list of parameters that can be extracted from simple characterisation tools and correlated/attributed to physical processes in the device. A common procedure in standard solar cells is the parametrisation of current–voltage curves. Fig. 1(a) shows the typical single-diode equivalent circuit used to describe the ideal electric behaviour of c-Si cells. For solar cells that do not behave ideally, this model is no longer valid and many authors have proposed modifications to fit experimental data. In particular in copper–indium–gallium–selenide (CIGS) solar cells and organic solar cells, sometimes a kink (that we will refer to as s-shape) is observed in the current voltage curves (Wagenpfahl et al., 2010) that cannot be modelled by the circuit in Fig. 1(a) (Romero et al., 2012). For a complete discussion on this s-shape *I–V* characteristic we remand to the works of Wagenpfahl et al. (2010) and Sandberg et al. (2014) and to the references within. Amongst the first proposed equivalent circuits, modifications were presented to the single-diode model for OPV as lumped parameters equivalent circuits, by substituting single diode with multiple diodes in parallel (Cheknane et al., 2008), or with complex not linear resistor blocks consisting of ideal diodes, a real diode and variable resistors (Mazhari, 2006). Unfortunately these solutions were again not suitable to simulate effectively s-shape behaviour. The circuit model that can simulate that behaviour was proposed by one of the authors (de Castro et al., 2010) (Fig. 1(b)) and later expanded by other groups (del Pozo et al., 2012; Romero et al., 2012; Garcia-Sanchez et al., 2013). It includes a second diode shunted by a resistor to simulate a region of the device (normally one of the interfaces) where charge accumulation leads to a change in the local electric field and as a consequence generates a charge injection process that is voltage dependent. When the current through the reverse second diode is small (good interface) the circuit of Fig. 1(b) reverts to that in Fig. 1(a). Although that reverse second-diode model could fit experimental data well within a limited voltage range, it relied on approximations to reduce the computational time and it did not include a term that would allow the current to increase again in forward bias after the s-shape. Recently Garcia-Sanchez et al. proposed an extension of that model replacing the resistance that shunts the reverse 2-diode by a third diode (Fig. 1(c)). The authors only solved the resulting equation for a few very specific cases where an explicit solution could be found. In those cases they could fit the full range of experimental current–voltage curve with s-shape. Clearly the

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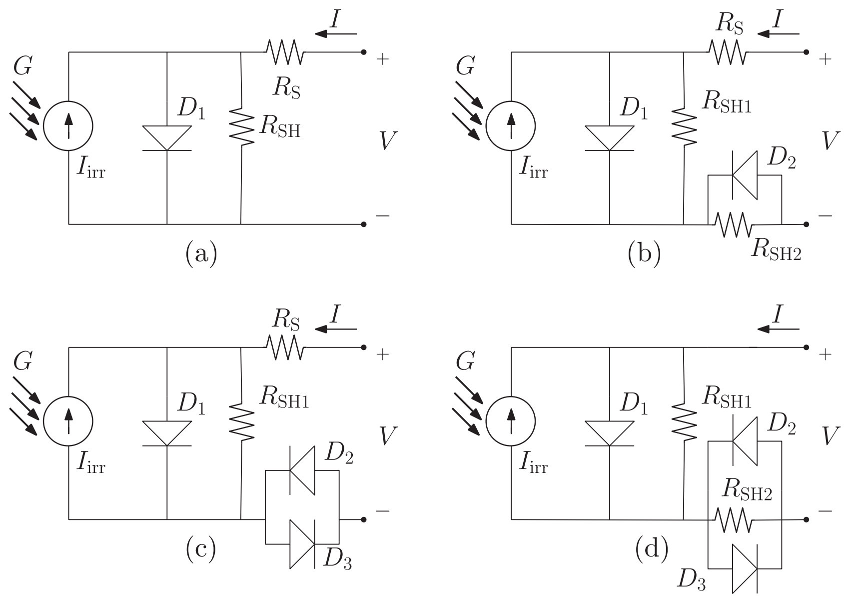

Fig. 1. One and multi diode equivalent circuit models for organic PV. (a) Traditional 1-diode model used for Si solar cells, (b) reverse 2-diode model (de Castro et al., 2010), (c) 3-diode model proposed by Garcia-Sanchez et al. (2013) that expands reverse 2-diode model to fit larger voltage range, and (d) new, generalised 3-diode model proposed in this paper.

validation and the choice of a model in favour of another is also linked to the possibility of finding physical parameters that are able to represent experimental data. This should be the solution of a well-posed identification problem. Unfortunately, for solar cells, one of the difficulties with fitting experimental data with equivalent circuits is that equations are transcendental and often the solution requires approximations. Iterations are also computationally expensive, which makes the procedure impractical when the number of curves to be analysed becomes very large. Therefore many authors rely on implications and approximations (Laudani et al., 2014; de Castro et al., 2010). A breakthrough was achieved in 2000 with the realisation that the Lambert W-function (Corless et al., 1996) could be used to provide an exact analytical solution to the current voltage curve of a diode with series resistance (Banwell and Jayakumar, 2000) and of a diode with both series and shunt resistance (Ortiz-Conde et al., 2000). Then, several authors have exploited the Lambert W-function to solve the current–voltage fitting problem for inorganic (Laudani et al., 2014; Jain and Kapoor, 2004) and organic photovoltaic devices (Jain and Kapoor, 2005; Romero et al., 2012). A few years ago Romero et al. proposed a solution for the reverse 2-diode model in Fig. 1(b). The solution found is very important since it expresses the relation *V*–*I* with a one-equation formula, but it has an important drawback due to the fact that it expresses voltage (V) as a function of current (I), whereas the measurements are usually done by setting the voltage and measuring the current. On the other hand, one of the main problems to be overcome when one tries to identify a model is to find the most suitable expression describing the model itself. Also in the case of organic solar cells this represents a significant issue which has led several authors in literature to use approximate formulas (de Castro et al., 2010) or complicated expressions based on circuital considerations (del Pozo et al., 2012).

This does not only influence the performance of the fitting routines, but also makes their accuracy difficult to evaluate. For this reason, in this work we present an improved methodology exploiting the use of exact one-equation formulas, different from what is available in the literature. We exploit the reverse 2-diode model and we propose a new, generalised 3-diode model (shown in Fig. 1(d)), to gain insight into the modelling and parametrisation of organic solar cell current voltage curves.

The paper is structured as follows: in Section 2 a short description of the used experimental data is reported; in Section 3 the one-equation model for 2-diode circuit (Fig. 1(b)) is presented, with a discussion on the limitations of the use of this model for the description of the current–voltage curves; in Section 4 the proposed 3-diode model is discussed and its advantages in the modelling OPV are demonstrated and validated by fitting a series of experimental organic solar cell curves with different degrees of s-shape; authors' conclusions follow in Section 5.

2. Measurements and experimental data

The solar cell devices were an enhanced bilayer of 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 (Castro et al., 2006; de Castro et al., 2010) ITO-coated glass coated with 50 nm of PEDOT:PSS (Aldrich, conductivity 1 S cm^{-1}) and subsequently coated with 50 nm of Al to serve as the cathode. Sample fabrication and characterisation was performed in inert N_2 atmosphere. Details of device sample preparation and characterisation were reported previously (Castro et al., 2006; de Castro et al., 2010). Current voltage curves were measured under inert N_2 atmosphere with samples exposed to 1000 W/m^2 simulated AM1.5G sunlight. Thermal annealing at different temperatures was used to reduce the s-shape as previously described (see Fig. 2 de Castro et al., 2010). In this manuscript we fitted curves of devices not annealed and annealed for 5 min at 120 °C, 150 °C, 180 °C and 200 °C. We refer to these samples as naIV100, a120C5min100, a150C5min100, a180C5min100 and a200C5min100, respectively. The experimental *I*—*V* curves for these data are shown in Fig. 2. It is possible to note that the samples, as prepared, show strong s-shapes.

3. The one-equation model for the two-diode circuital representation of an OPV

In this paragraph we describe how to obtain the one-equation model representing the mathematical relation between voltage *V*