Reliable extraction procedure of parameters for the modeling of organic photovoltaic cells

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INTRODUCTION

The organic photovoltaic (OPV) has been a topic of high interest in the past years, with solar cells reaching conversion efficiencies above 10% [1]. For such performance, the active layer of the cells consists of a blend of donor and acceptor organic materials forming a structure known as bulk heterojunction (BHJ).

The morphology of these solar cells is known to have a significant effect on their performance [2]. However, the main models used to interpret and predict experimental results are restricted to one-dimensional approaches. Therefore, in order to investigate the effect of the charge transport anisotropy coming from the active layer morphology, we developed a two-dimensional model reproducing an ideal BHJ structure, made of two interpenetrating combs of donor and acceptor materials (Fig. 1). As this 2D model involves parameters that are not directly accessible by experimental measurements, we developed a suitable extraction method to get them.

MODEL

The model is based on the charge generation mechanism, which is depicted in Fig. 2. In this approach, the generation of free charge carriers requires an intermediate state, called Charge Transfer state.

The electrical characteristics of an OPV cell are obtained by solving a Poisson equation coupled to modified drift-diffusion equations. In addition, a specific boundary condition is set up to take into account the mechanisms that occur at the interface between the two organic materials [3]. The final model was successfully validated by comparison with experimental characteristics of a standard P3HT:PCBM cell, for various light intensities [4].

The extraction of the unknown parameters is achieved by means of a specific Markov chain Monte Carlo (MCMC) fitting procedure [5]. Indeed, more classical fitting procedures using Levenberg-Marquardt algorithm are no longer reliable for the number of parameters considered here (up to 20 when some geometrical parameters are concerned). Moreover, using this MCMC approach, we obtain valuable statistical information on the validity of each parameter extracted.

EXPLOITATION

The extraction procedure was applied on the experimental measurements used in Ref. [4]. The resulting statistics provide the correlations between the different parameters, as shown by the six correlation diagrams in Fig. 3, which correspond to the four main parameters of the model.

In Fig. 4, the histograms associated with the occurrence of the various values of these four parameters are plotted (coming from the projection of the correlation points on the four corresponding axes). They directly reflect the probability distribution of each parameter. Some peaks, more or less well defined, can be identified on these histograms.

By selecting a set of points following a linear trend within the correlation plot of the electron mobility μ_n *vs.* the effective density of state N_c (first plot in Fig. 3), we are able to identify the corresponding parameters within the other correlation plots (red dots in Fig. 3).

This selection, which was echoed in red on the histograms of Fig. 4, indicates that the parameter set 1 (thick solid lines) corresponds to one of the most probable. Furthermore, with this method, we can study other suitable sets of parameters. Indeed, the set 2 (dashed lines in Fig. 4) corresponds to secondary peaks for most of the parameters, and both sets 1 and 2 can perfectly fit the experimental characteristics, as shown in Fig. 5 for J-V curves. Consequently, the probability distribution of the

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parameter values gives a criterion for selecting the best fitting set of parameters.

CONCLUSION

The 2D modeling of OPV cells leads to a complex system with a large number of unknown physical parameters. The MCMC fitting procedure has the advantage of providing some information about the dependence between the extracted parameters, and it paves the way for the study and validation of various mechanism hypotheses in less known OPV cells, which is impossible with classic fitting procedures.

This methodology can also be applied to other applications having a large number of fitting parameters.

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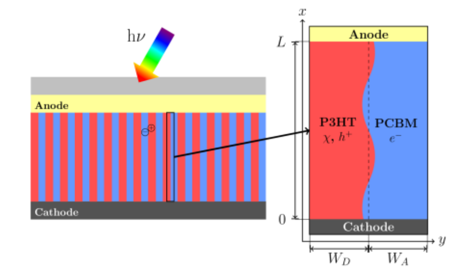

Fig. 1. Diagram of the layer stack of a typical OPV cell with an ideal BHJ active layer (left). Schema showing the elementary structure of the modeled active layer and the specifications of the geometrical features (right).

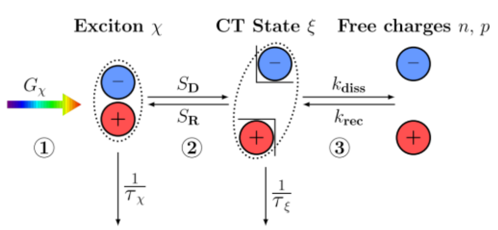

Fig. 2. Diagram presenting the charge generation mechanism implemented in our 2D OPV cell model. The various reaction rates between species are indicated, starting from the creation of exciton from photon up to free charge carriers.

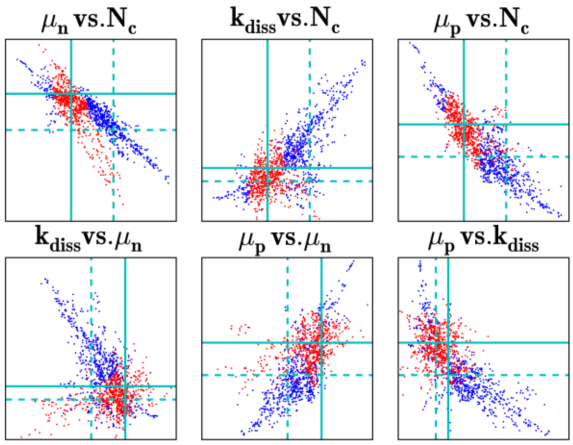

Fig. 3. Correlation plots between the four main parameters, obtained from the statistical data of the extraction procedure. The solid and dashed line reticles refer to the parameter sets 1 and 2 of Fig. 4, respectively.

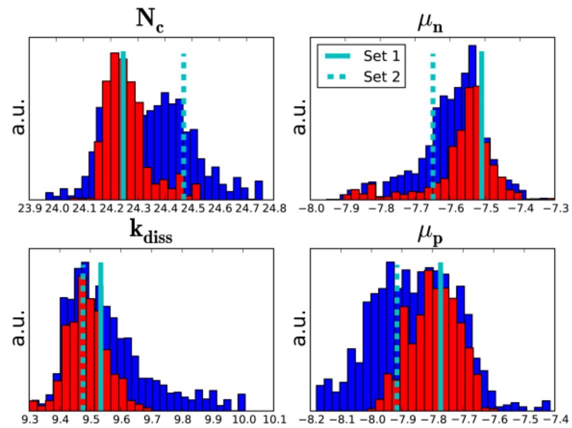

Fig. 4. The blue histograms correspond to the projection of all the points of Fig.3 over one parameter, in a common logarithmic scale. The red histograms are only associated with the red selected points of Fig. 3. The parameter sets 1 and 2 are indicated by solid and dashed lines respectively.

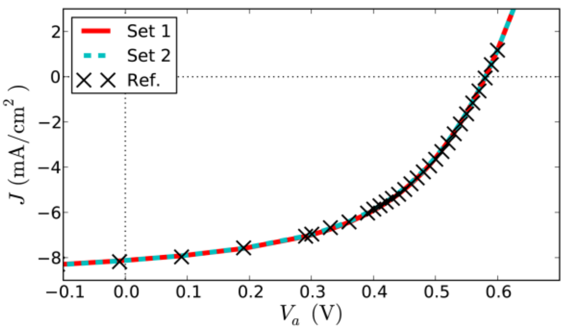

Fig. 5. Current density vs. applied voltage curves for the reference experimental characteristic (black crosses), the parameter set 1 (solid red line) and the parameter set 2 (dashed cyan line).