Numerical drift-diffusion modeling of organic solar cells in comparison with experimental data series

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***Abstract*—Recently, much effort has been put in the simulation of charge transport in organic materials and more and more sophisticated models with an increasing number of parameters are developed. In this paper, we show which models are necessary and applicable for the drift-diffusion modeling of IV curves of multilayer solar cells. For comparison to experiment, a data series of small molecule organic solar cells comprising several materials, architectures, and thicknesses of layers is used. The model is chosen as simple as possible to reduce the number of parameters and to allow for the identification and accurate investigation of the key processes in detail. As exemplary result, the spatial exciton generation profile is examined within the active blend layer: It does not only influence the short circuit current, but also the fill factor and open circuit voltage at constant short circuit current, especially in the case of imbalanced mobilities. In another example where interfacial barriers are present, broadening of the energy levels due to disorder has to be taken into account to describe the IV curves showing S-Shape like behavior with realistic parameters. Transient measurements of extraction barrier devices show indeed an accumulation of charge carriers as predicted by simulation.**

I. Introduction

The performance of organic solar cells has increased rapidly in the last years. This progress until now is mainly based on trial-and-error and optimization experiments. However, there have been many models developed and refined, describing charge carrier transport, injection, and exciton separation in organic materials [1]. The Gaussian disorder model is very common and Monte Carlo simulations are done to describe morphology and charge transport in organic layers [2]. However, a description of experimental data of devices is still a considerable challenge. On the one hand, many of the models are too complex to use them to describe a complete solar cell stack. On the other hand reliable, reproducible experimental data series are rare. We try to face this issue by using a large series of samples and a drift-diffusion model, which is capable to reproduce trends qualitatively and in the correct range of used parameters without focusing on an exact fit of the IV curve. Showing the capability of the simulation we point out two following phenomena in this contribution, which are not yet well accounted for in literature.

II. Model

The simulation is based on a one dimensional drift-diffusion model [3], taking into account the results from microscopic modeling. The basic model is comparable to Ref. [4]. Field-, charge carrier density-, and temperature dependent mobilities can be used to describe the hopping nature of charge transport. To account for disorder in the amorphous layers a Gaussian broadened density of states and Fermi-Dirac statistics with a generalized Einstein relation are implemented. Excitons can be modeled by diffusion and at a heterointerface by a field dependent separation term. Trap distributions can be included. The grade of sophistication used to model the presented IV curves depends on the requirements for a good description of experimental data. It is furthermore dominated by the materials used.

III. Example I: Role of spatial generation profile

It is well known that optical interference effects have to be considered in organic solar cells with layer thicknesses of some 10s of nanometers. This is commonly done by a transfer-matrix algorithm and gives good results in comparison to absorption measurement data. For the electrical simulation, the spatial exciton generation profile (which equals the charge carrier generation profile in a homogeneously mixed bulk heterojunction) is thought to be of minor importance and usually an average value is used. By using the exciton generation profile from the optical model as charge carrier generation profile in the absorbing blend, we show that this effect has to be taken into account, especially for monochromatic illumination, where the generation profile is varying considerably (Fig. 2, insets). In this case and in combination with imbalanced mobilities in the blend layer (slow holes have to move from right to left and fast electrons from left to right) not only the short circuit current but fill factor and open circuit voltage (V_{oc}) are changed due to different overall recombination, even if short circuit current is adjusted to be the same in experiment and simulation (see Fig. 1, 2). In device I, generation occurs mainly near the anode (left), in device II with C60 that acts as buffer and additional absorber layer mainly near the cathode. The effect is stronger for blue color, where some excitons from the C60 layer diffusing into the blend layer cause a high charge carrier generation at x = 70 nm. Because hole mobility ($\mu_p \approx 5 \times 10^{-5}$ cm^2/Vs) is much lower than electron mobility ($\mu_e \approx 10^{-3}$ cm^2/Vs), the overall recombination is changed between the two solar cells and colors. Using further samples with other geometries, this effect is proven and found to be independent on the illumination color itself.

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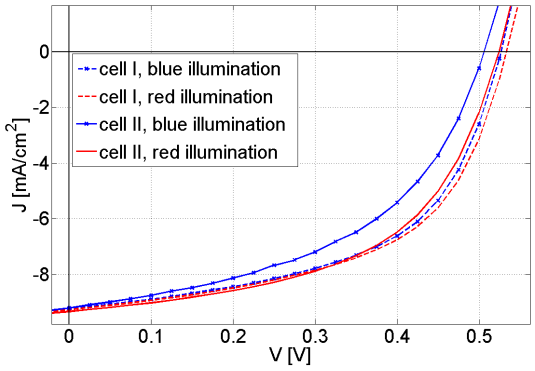

Fig. 1. Experimental IV curve of two solar cells, illuminated with a blue and red LED. Device I: ITO/p-DiNPB(25 nm)/ZnPc:C60(45)/BPhen(6)/Al, Device II: ITO/p-DiNPB(25)/ZnPc:C60(45)/C60(60)/BPhen(6)/Al.

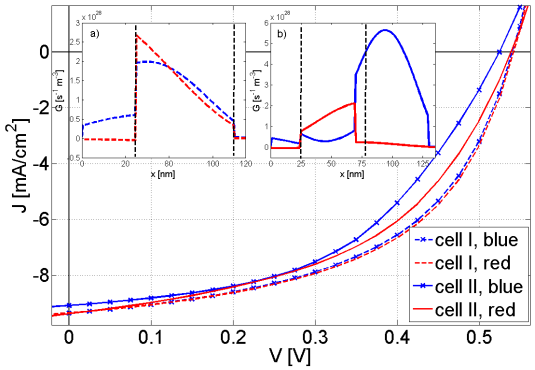

Fig. 2. Simulated IV curves of devices from fig. 1, Most important input parameters: LED spectra, mobilities $\mu_e = 10^{-3}$ cm^2/Vs, $\mu_p = 5 \times 10^{-5}$ cm^2/Vs. exciton diffusion length in C60 10 nm. Insets show for device I (a) and device II (b) (x = 0 at ITO/p-DiNPB interface) exciton generation profiles with maxima shifting from the left to the right from device I to II. The active region is found between the vertical lines.

IV. Example II: Interfacial Barriers

The influence of barriers at the contact on the IV curve is still under discussion. Here, barriers for holes are investigated by a variation of hole transport layer and donor material in a flat heterojunction solar cell (insets of Fig. 3). With experiment and simulation we show, that V_{oc} is not defined by the workfunction of the p-contact in a pin-solar cell with wide-gap charge transport layers, which act as semipermeable membranes. It is dominated by the HOMO level of the donor and hence the effective transport gap at the heterointerface, whereas the FF and the shape of the curve are influenced by barriers. Both, injection and extraction barriers result in S-shaped IV curves (Fig. 3). When analyzing simulation data of charge carrier density and electric field profiles in the solar cell, these effects can be explained by changed directions of drift and diffusion currents. Simulations show further, that a barrier-lowering expression should be included (Fig. 4). Also disorder plays a significant role in this case, increasing the barrier crossing probability. The accumulation of holes, which is predicted by simulation in the case of extraction barriers, is proven by photocurrent transient data. Transient simulations concerning this issue are currently under investigation.

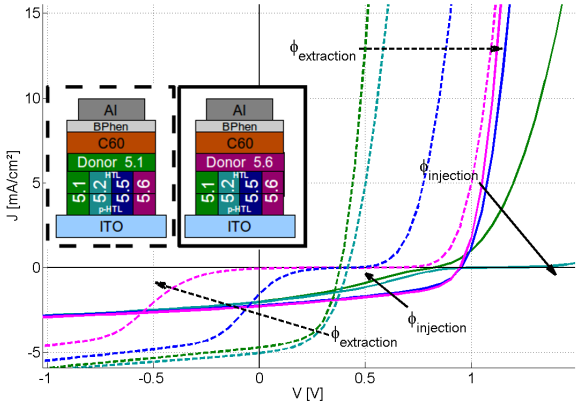

Fig. 3. Experimental data of eight cells. Stacks are shown in insets. As HTL/ donor materials ZnPc (HOMO 5.1 eV), MeO-TPD (5.2), α-NPB (5.5), and BPAPF (5.6) are used. Values from UPS data with error of $\pm$0.1 eV.

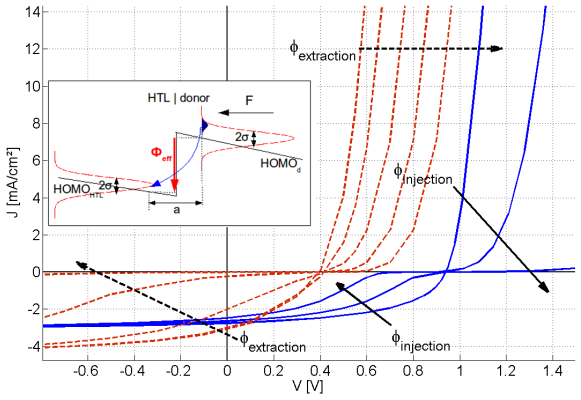

Fig. 4. Simulation data of barrier devices. Barriers for injection 0, 0.2, 0.4 eV, for extraction 0.2..0.6 eV, average hopping distance a = 1 nm, width σ = 150 meV. The inset shows a schematic sketch of the model in case of an extraction barrier for holes with applied field

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