The Influence of Transport Layers on the Performance of Organic Solar Cells Studied by Drift-Diffusion Model

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Abstract—**The existence of a hole transport layer (HTL) and an electron transport layer (ETL) in organic solar cells (OSCs) was considered in the drift-diffusion model (DDM) in a simplified way: domain for solving the DDM equations was divided into three subdomains corresponding to the HTL, an active layer (AL) and the ETL. Different material parameters such as electron and hole mobility, dielectric permittivity, recombination rate, and absorption coefficient, characterizing each layer, were applied for each subdomain. The Dirichlet boundary conditions were used on electrode/transport layer (TL) interfaces. The boundary conditions on TL/AL junctions were omitted so that TLs were accounted only through each layer material parameters. The DDM simulations were carried out by assuming photogeneration only in the AL. To examine the validity of our approach, dependencies of power conversion efficiency, fill factor, open circuit voltage and short circuit current density on the mobilities of majority and minority carriers in the HTL and ETL as well as on the recombination rates in these layers were determined and it was checked whether they meet the expected trends. Further, the current density–voltage (J-V) curves were simulated using the DDM which accounts for the TLs and the standard DDM not taking into account the TLs for ITO/PEDOT:PSS/P3HT:PCBM/LiF/Al solar cell, and obtained results were compared to the experimental ones from literature. Simulated J-V curves matched well the experimental data when TLs were included.**

Keywords—numerical simulation, organic solar cells

I. INTRODUCTION

Organic solar cells (OSCs) known for its flexibility, cost effectiveness and potential for roll-to-roll processing, have been recognized as part of emerging photovoltaics by the National Renewable Energy Laboratory's yearly best research efficiency chart since 2001 [1]. The power conversion efficiency (PCE) of OSCs has been significantly improved in the past few years, with the maximum confirmed PCE of 19.2%[1, 2]. The progress so far has been carried out by the development of new materials and mixtures as well as new device structures. However, to fully exploit the potential of OSCs, it is necessary to develop an adequate and comprehensive physical model that will serve as a guide for further performance enhancement.

It is well known that the hole transport layers (HTLs) and electron transport layers (ETLs) significantly improve the performance of OSCs and therefore, they are indispensable parts of their structure [3, 4]. However, within the framework of drift-diffusion models (DDMs) used for OSC modelling, the existence of these layers is not taken into account [5].

II. THE MODEL

The role of transport layers (TLs) is to improve the transport of majority carriers and, if possible, to hinder the transport of minority carriers to electrodes. Also, TLs reduce energy barriers between the active layer and electrodes (energy level alignment) leading to more efficient charge carrier extraction and reduction of recombination losses. Having these roles of TLs in mind, we can try to avoid solving the set of DDM equations separately in each layer of OSC. The enhanced majority carrier transport near the electrode can be simply modelled by using a higher majority carrier mobility in the region of HTL and ETL than in the active layer (AL). Also, the energy level alignment is easily modelled by assuming low or zero injection barriers on electrodes' contacts.

The DDM considered in this paper is the same as in Ref. [6] with the assumption that all surface recombination velocities tend to infinity and hole and electron injection barriers are zero. In this way, the boundary conditions (BCs) were reduced to Dirichlet BCs. This was applied to the so-called external BCs on the electrode/TL interfaces. The photogeneration rate profile was determined based on the Beer-Lambert law and the photogeneration was assumed to take place only in the AL. The domain for solving the DDM equations was divided into three subdomains corresponding to the HTL, AL and ETL.The absorption coefficient (α), dielectric permittivity (ε_r), electron and hole mobilities (μ_n, μ_p) and recombination rate reduction coefficient (ξ) were considered to be real and different for each layer. We did not set any internal BCs at the AL/TL junctions and the existence of TLs was included in DDM calculations only through material parameter inhomogeneity.

III. RESULTS AND DISCUSSION

Based on DDM used in this paper we have determined the dependences of power conversion efficiency (PCE), fill factor (FF), open circuit voltage (V_{oc}) and short circuit current

density (J_{sc}) on majority and minority charge carrier mobilities in the ETL (μ_n^{ETL} and μ_p^{ETL}), and in the HTL (μ_p^{HTL} and μ_n^{HTL}) as well as on ξ. The obtained dependencies were in agreement with the expected trends. As an example, the J-V characteristics calculated for different μ_n^{ETL} and μ_p^{HTL} are presented in Figs. 1, and 2, respectively. PCE and FF dependences on μ_n^{ETL} and μ_p^{HTL} are given in corresponding Insets of Figs 1 and 2. As expected, PCE is improving with increasing μ_n^{ETL} and μ_p^{HTL}, and FF stays approximately the same. The appropriate behaviour of V_{oc} and J_{sc} with a change in μ_n^{ETL} and μ_p^{HTL} can be deduced from J-V characteristics shown in Figs.1 and 2, respectively.
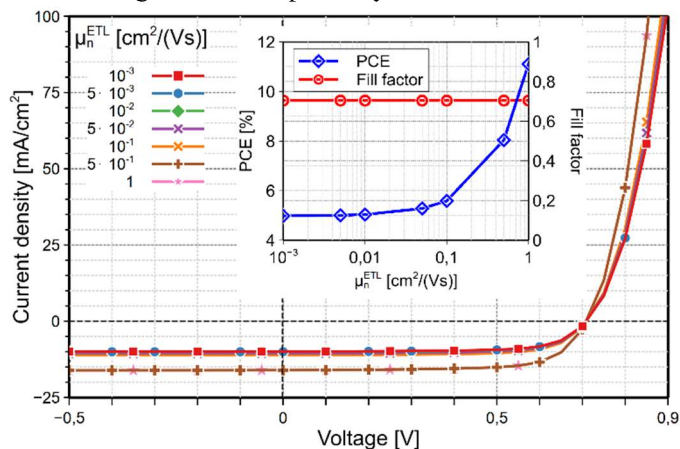

Fig.1. Simulated J-V characteristics for different μ_n^{ETL} PCE and FF dependences on μ_n^{ETL}- Inset.
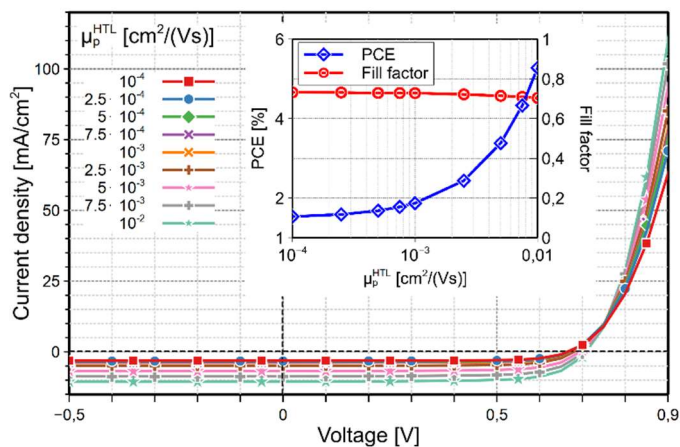

Fig.2. Simulated J-V characteristics for different μ_p^{HTL} .PCE and FF dependences on μ_p^{HTL}- Inset.

Furthermore, the simulated J-V curves obtained by the DDM including the TLs (DDM_TLs) and the standard DDM not taking into account the TLs (DDM_S) are compared with the experimental J-V characteristic for ITO/PEDOT:PSS/P3HT:PCBM/Al solar cell (Fig. 3) taken from [7]. The material constants used in simulations are given in the Inset of Fig. 3 and their values are realistic for the particular materials. According to Fig. 3 the DDM_TL reproduces well the experimental data while the DDM_S shows a notable disagreement with the experimental J-V curves.

The performance of organic solar cells is extremely sensitive to the choice of the ETL and HTL, their thicknesses and the electrical and optical constants of the layers as it is indicated by our model. Considering the boundary conditions at the AL/TL interfaces will be the subject of our further work.
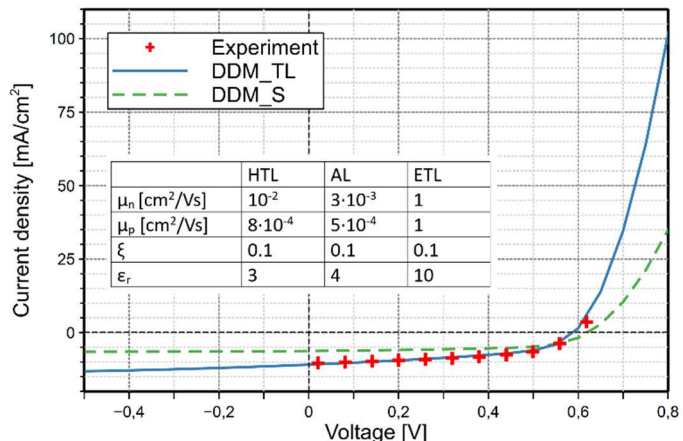

Fig 3. The ITO/PEDOT:PSS/P3HT:PCBM/LiF/Al solar cells J-V characteristics simulated by DDM_TL and DDM_S and compared with measured J-V characteristics taken from Ref. [7].

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