Current-Voltage Characteristics Simulations of Organic Solar Cells Using Discontinuous Galerkin Method

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***Abstract*–The steady state drift-diffusion model (DDM) of organic solar cells that considers the surface recombination processes for majority and minority carriers, as well as their thermionic emission on both electrodes, is presented in this paper. When the full Robin boundary conditions (BCs) and the popular finite difference method with Schaffeter-Gummel discretization (FDSG) were applied, significant instabilities were observed when surface recombination velocities (SRVs) for majority carriers on one or both electrodes were reduced. To analyze this problem and perceive the independent impacts of electron and hole contact processes, the model was simplified by assuming a constant electric field in the device and by solving the electron and hole continuity equations separately. The stability of numerical DDM solutions obtained by the FDSG and Discontinuous Galerkin (DG) methods for three different types of BCs (Dirichlet and two mixed BCs) was examined. The DG method showed a better stability when majority carriers SRVs were reduced. The current density versus voltage (*J*-*V*) characteristic calculated by the DDM with Dirichlet BCs using the DG method was compared to the measured ITO/PEDOT:PSS/P3HT:PCBM/Al solar cell *J*-*V* curve for the model validation.**

I. Introduction

Organic solar cells (OSCs) are a promising technology because they offer advantages of being lightweight and flexible, and have a low manufacturing cost for large-area production [1]. Their power conversion efficiencies have now reached 17.5% [1]. Still, the potentials of OSCs have not been completely exploited due to the lack of an adequate physical model that describes their operation. The OSCs are usually modelled by the drift-diffusion model (DDM) [2], which is numerically solved by either finite difference (FD), finite volume (FV), or finite element (FE) method using Schaffeter-Gummel (SG) discretization [3]. The frequently used boundary conditions (BCs) in the DDM are the Dirichlet or mixed (which uses homogenous Neumann conditions for minority and Dirichlet conditions for majority carrier concentrations) [2, 3]. It was shown that surface processes on electrode contacts in OSCs have a significant impact on their performance [4]. The influence of surface recombination for majority and minority carriers, as well as their thermionic emission on electrodes, is modeled by introducing the full Robin boundary conditions in the DDM. The numerical methods mentioned above do not give solutions in a complete range of possible majority and minority surface recombination velocities (SRVs).

II. Models

The DDM considered in this paper is the same as in [5] including the form of BCs, whereby the majority carrier injection barriers were assumed to be zero. To avoid complexities of the problem and to enable a separate analysis of the effect of electron and hole BCs on the steady state solution, some simplifications were introduced. First, we assumed the electric field to be constant. Second, the electron and hole continuity equations were decoupled by taking the electron bimolecular recombination velocity to be $R_n = \gamma n^2$ and analogously for holes $R_p = \gamma p^2$, where γ is the Langevin recombination constant, and n and p are electron and hole densities, respectively. For the numerical solution, two different methods were used.

In DDM_FDSG model, we applied the FD method with the SG discretization (FDSG), which uses exponential approximation of carrier densities at midpoints of a one-dimensional mesh, with Newton algorithm implemented to solve the discretized system [5].

The other model was the DDM_DG in which the Discontinuous Galerkin (DG) method [6] was used. To solve the simplified model consisting of one nonlinear second-order differential equation (electron or hole continuity equation), we first decoupled the equation to obtain a system of 2 first-order equations. For discretization, we used a local DG scheme with Lagrange polynomials at Legendre-Gauss-Lobatto nodes of degree 8 as testing functions and discrete inner product. The Lax-Friedrichs numerical flux for the drift term and the local DG flux for the diffusion term were used as in [6].

III. Results and discussion

The electron current density versus voltage J_n-V, and the hole current density versus voltage J_p-V characteristics, were calculated by using the DDM_FDSG and DDM_DG models. The calculations were conducted for three different types of BCs: Dirichlet, mixed_1 (minority Robin and majority Dirichlet), and mixed_2 (majority Robin and minority Dirichlet). In the Robin BCs, SRVs for majority and minority carriers were categorized as

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large (L), medium (M), and small (S), the same as in [4] and [5] except that the drift current for both electrons and holes was taken to be dominant in this paper. The results are presented in Fig. 1. As it can be seen from Figs. 1 (a) and (b), the DDM_FDSG model showed significant instability for the mixed_2 boundary conditions when majority carrier SRVs were reduced (M or S values). For M values, the J_n-V and J_p-V curves predicted by the DDM_FDSG model are unexpectedly large in the first quadrant, while for S values the calculation diverges and gives broken J_n-V and J_p-V curves. The DG model in the case of the mixed_2 BCs is stable for M and S SRVs values used in calculations presented in Figs. 1 (a) and (b). The Dirichlet and mixed_1 BCs gave nearly the same prediction of J_n-V and J_p-V characteristics depicted in Fig. 1 (c). In this case, the calculations were stable for the DDM_FDSG model in a wide range of SRVs. The parameters used in the calculations correspond to the ITO/PEDOT:PSS/P3HT:PCBM/Al solar cell taken from [5]. In Fig. 2, the measured J-V characteristic of the same solar cell is compared to the total (J_n+J_p) current density versus voltage characteristic determined by the DDM_DG model with the Dirichlet BCs. The agreement between the calculated and experimentally obtained J-V curves is very good, which validates the model.

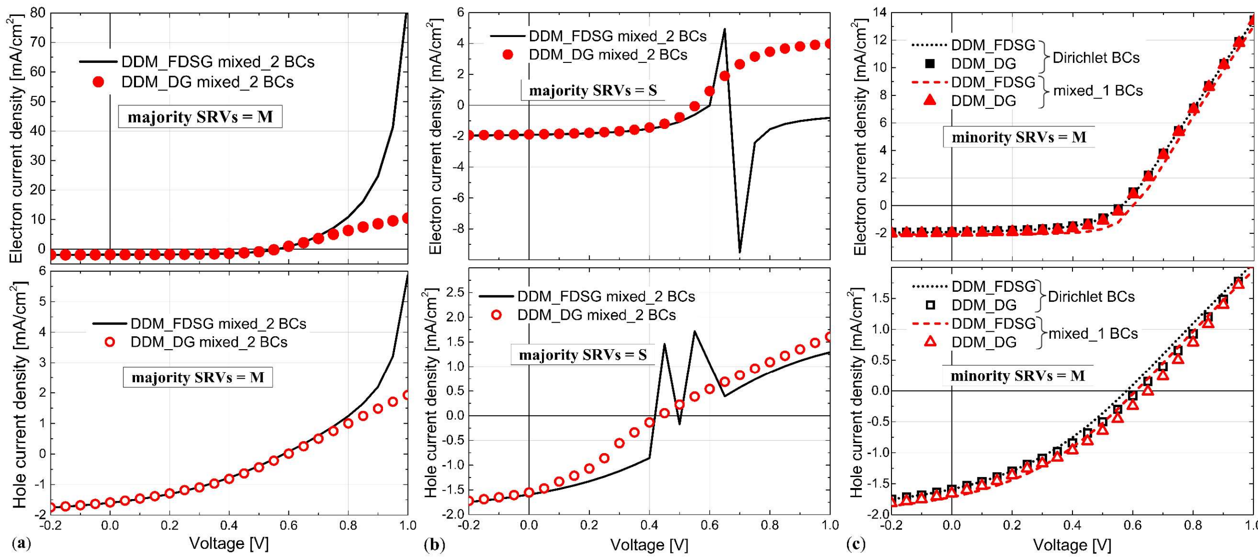

Fig.1. J_n-V and J_p-V curves simulated by DDM_FDSG and DDM_DG models for (a) mixed_2 BCs with M SRVs values, (b) mixed_2 BCs with S SRVs values, and (c) Dirichlet and mixed_1 BSs with M SRVs values.

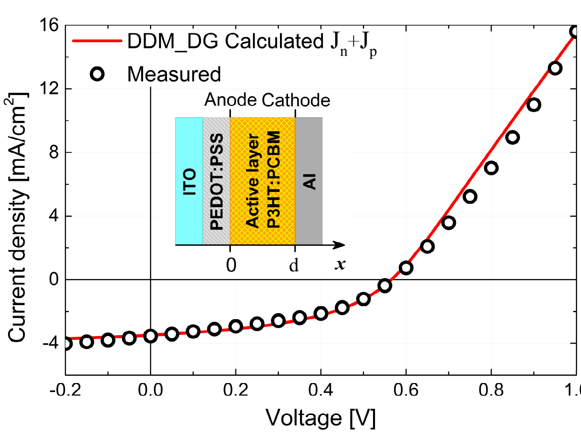

Fig 2. The ITO/PEDOT:PSS/P3HT:PCBM/Al solar cells J-V curves, measured and simulated by the DDM_DG model with Dirichlet BCs. Shematics of the device – Inset.

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