Built-in electric field in irregular morphologies of bulk-heterojunction solar cells

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***Abstract*—This paper theoretically analyzes the built-in electric field distribution in bulk heterojunction solar cells. The approach proposed leads to explore the impact of regular and irregular morphologies on the performance of these devices. The width of the depletion region at the donor-acceptor interface is set by the doping concentration. The proposed analysis resulted in the best behavior for an interdigitated structure and the worst for the planar heterojunction cell as expected.**

Keywords—Organic semiconductor, bulk-heterojunction, irregular morphology

I. Introduction

Organic semiconductor materials having short exciton diffusion length lead to inefficient solar cells when they are used within the active layer with a planar heterojunction [1]. This is because, only the excitons generated within the diffusion length from the heterojunction can be dissociated into charge carriers and contribute to photocurrent. The bulk heterojunction (BHJ) architecture, which comprises an interpenetrating network with nanoscale phase separation between a donor and an acceptor materials, has been intensively used as the approach to overcome exciton dissociation [2]. The BHJ structure creates a larger interface area and smaller exciton to interface distances than in the planar heterojunction, so that an electric field in the vicinity of the interfaces of donor and acceptor materials is distributed throughout the volume of the active layer and a more effective charge separation is achieved. The ideal morphology for the active layer is the interdigitated heterojunction structure, where vertically aligned donor nanopillars are surrounded by the acceptor materials with nanoscale phase separation, or vice versa. However, the implementation of the ideal interdigitated structure is difficult. Instead, a mixed solution deposition method is the most extensively used because is not expensive and high power conversion efficiencies can be achieved. In this case, active layers with irregular morphologies are obtained since the random mixing nature of the donor and acceptor during solution processing.

When bulk heterojunctions are considered, an optimum distribution of the built-in electric field throughout the volume of the active layer is needed, to balance exciton dissociation and transport of electrons and holes. Having a model to evaluate the distribution of the built-in electric field for regular (interdigitated heterojunction structure) and irregular morphologies of the active layers is critical to understand and improve the performance of BHJ solar cells.

The one-dimensional approach is the model that has been largely used to calculate the electrical behavior of BHJ solar cells. This model assumes that the internal nanostructure of the active layer is one semiconductor with properties derived from the two materials of the blend [3], and predicts that the máximum intensity of the electric field occurs near the electrodes. However, this model does not take into account the effects of the morphology of the blend, since it only considers an effective-medium. Currently, there are few theoretical methods to analyze the relationship between morphology and electrical behavior of solar cells [4]. That is why it is not yet clear how the ideal morphology of a bulk heterojunction should be.

In order to explore bulk-heterojunction morphologies, here we propose an approach that takes into consideration not only the electric field that occurs near the electrodes but also that which is built at the donor-acceptor interface.

II. Computational Details

Since our goal is to explore the generic impact of morphology on the performance of BHJ solar cells, we arbitrarily consider a donor and acceptor materials, whose parameters are shown in Fig.1 and Table I, and a simple algorithm that generates random disordered morphologies with radial growth donor/acceptor phases [5].

To simulate correctly the behavior of BHJ solar cells, we consider that unintentional electrical doping is present and has a dominant effect on the built-in electric field at the donor-acceptor interface. The doping concentration generates a depletion region whose width can be controlled. The transport of carriers on the simulated morphology is modeled by the drift–difusión formalism. We assume a bimolecular recombination with a direct recombination constant, and an uniform optical absorption profile [6].

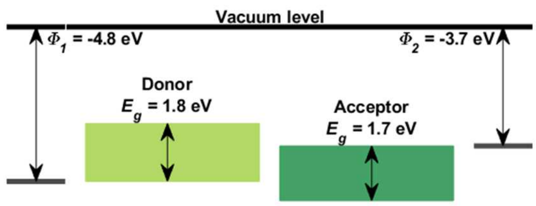

Fig. 1. Band energies of the herojunction used to simulate.

TABLE I. Parameters used in the 2D drift-diffusion simulation.

Parameter	Numerical value
Dielectric contact	1.5
Effective density of states	2.5×10^{21} cm^{-3}
Electron and hole mobilities	2.5×10^{-3} cm^2/V-s
Generation rate	2.7×10^{21} cm^{-3}.
Direct recombination constant	1×10^{-10} cm^{3}s^{-1}
Doping concentration	2.5×10^{18} cm^{-3}

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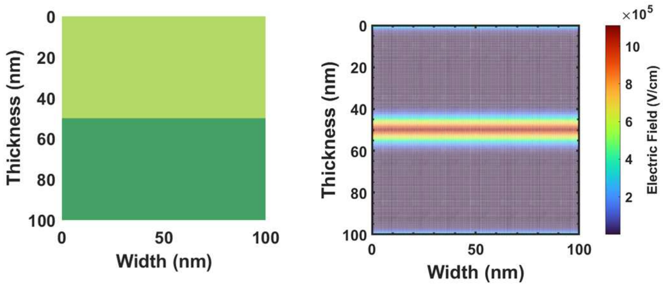
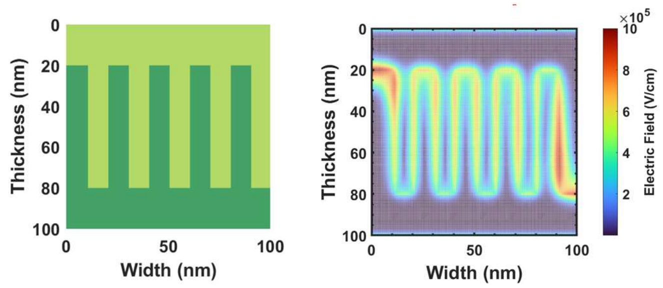
III. RESULTS

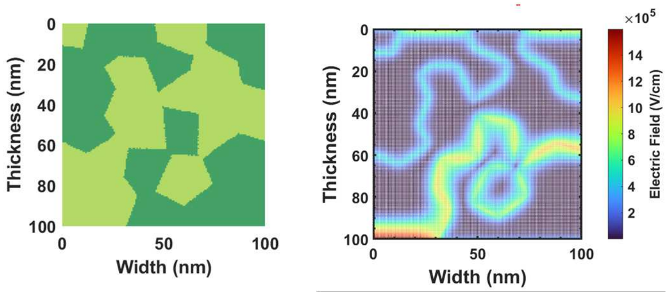
With the model described in the previous section, we calculate the electric field of BHJ solar cell as a function of the morphology. In Fig. 2, active layers with regular and irregular morphologies and their respective electric fields under short-circuit and illuminated condition are shown. For all cases, we note that the maximum intensity of the electric field is at the interface. From Fig. 2*a*, it can be seen that the depletion region at the heterojunction is almost 20 nm wide. It is worth mentioning that the depletion region width can be modulated by doping concentration. In Fig. 3 the current density-voltage characteristics for simulated morphologies are shown. As it was expected, our approach shows that the best performance is obtained for the interdigitated heterojunction with a maximum power of 2.3 mW/cm^2.



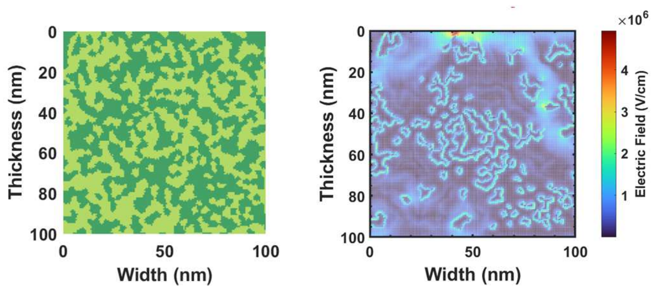
a) Planar heterojunction structure and its electrid field.



b) Interdigitated heterojunction structure and its electrid field.



c) Irregular morphology with large domain size and its electric field.



d) Irregular morphology with small domain size and its electric field.

Fig. 2. Simulated morphologies with their respective electric fields.

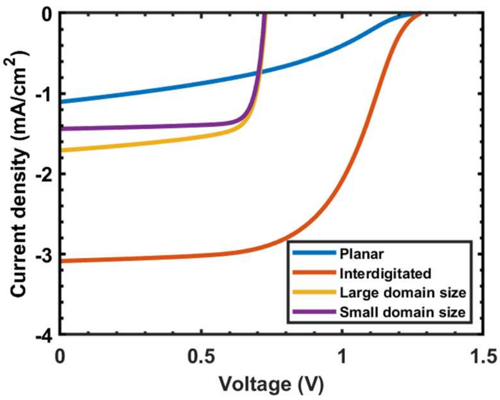


Fig. 3. Current density−voltage characteristics of bulk heterojunction solar cells with different morphologies.

Unlike the irregular morphologies, the planar heterojunction and the interdigitated structure have large open-circuit voltages, 1.27 V, but with low fill factors, 37.4% and 58.3%, respectively. It is interesting to note that the open-circuit voltage does not depend on the average domain size when the morphology is irregular, 0.72 V, however, the short-circuit current density is lower when the domain size is reduced, 1.44 mA/cm^2. It can be explained by the lack of continuous pathways that affects the transport of electrons/holes towards the corresponding electrodes when the average domain size is small.

IV. CONCLUSIONS

In this work, we analyze morphologies in BHJ solar cells taking into account the electric field that is built throughout the active layer. In this approach, the width of the depletion region can be modulated by doping concentration. It provides a better physical description than the effective-medium model. Although we choose arbitrary semiconductor materials to illustrate our approach, the conclusions are general and should apply to any heterojunction.

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