An algorithm to generate two-dimensional morphologies of organic solar cells

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***Abstract*—In this paper we show an algorithm that generates the morphology of a bicontinuous interpenetrating network between donor/acceptor semiconductors in the active layer of an organic solar cell. The domain size, mixing ratio and the resolution can be controlled by the algorithm. Also, we present the comparison of the simulated morphology with experimental results found in the literature. This algorithm does not require a high computing capacity and the time consuming is low.**

Keywords—morphology, active layer, bulk heterojunction, organic solar cell, simulation, algorithm.

I. INTRODUCTION

Organic solar cells (OSCs) present attractive features, for example: transparency, flexibility and low-cost development. The active layer of the OSC, where the photovoltaic effect occurs, is composed by two organic semiconductors materials (donor and acceptor).

One of the main problems that the OSCs face is the inferior power conversion efficiency (PCE) in comparison to conventional, inorganic photovoltaic technologies. Remarkable improvement in efficiency of OSCs has been achieved during the last decade. While the first devices had a PCE less than 1%, today new OSCs with 11.2% of efficiency have been reported [1]. One of the key innovations has been the bulk heterojunction (BHJ) used in the active layer, which is obtained by mixing donor and acceptor materials to form a bicontinuous interpenetrating network. However, due to the complexity, the physical mechanisms that occur inside the active layer are still not fully understood. Great efforts have been made for gaining structural insight into the effect of the BHJ morphology, the particular nanostructure of the BHJ, on the PCE of the OSCs. There are different experimental results reported in the literature that have shown the change of morphology by using different concentrations ratio [1] or different kind of solvents [3], among others [4] and the morphology-PCE relationship. In the same direction, there are several theoretical works in the literature that simulate the morphology in the active layer of an OSC to analyze the effect on the efficiency. For example, the Kinetic Monte Carlo (KMC) [5], that needs the use of a supercomputer, and the Dissipative Particle Dynamics (DPD) method [6], that makes the three dimensions simulation. However, these methods are time consuming and the computational cost is high due to the complex models based on single microscopic processes.

In this work, we propose an algorithm that generates two-dimensional disorder morphologies using a simple and fast method to grow the donor/acceptor phases. This algorithm will allow in future works the analysis of the distribution of the electric field within the active layer.

II. IRREGULAR MORPHOLOGY METHODOLOGY

A mesh discretization of the continuous active layer is carried out. Each cell of the mesh represents a portion of the active layer. The proposed algorithm consists of deciding for each cell if it is either donor or acceptor material. A matrix with m rows and n columns was used to represent each cell of the mesh. Setting the size of the matrix, the number of rows and columns, the resolution of the morphology can be controlled.

First, the number of domains is defined. For each domain, an initial position of growing is assigned randomly in the matrix (Fig.1*a*). In order to avoid agglomeration, there must be a minimum distance between initial points, L_{min}. Then, each domain starts growing in a radial form, with different growing rates (Fig.1*b*). The growth domains must fill each element of the matrix and stop increasing in size until they reach either another growth domain or one edge of the matrix (Fig.1*c*). Finally, the algorithm randomly decides for each domain if it is donor or acceptor material considering the mixing ratio (Fig.1*d*).

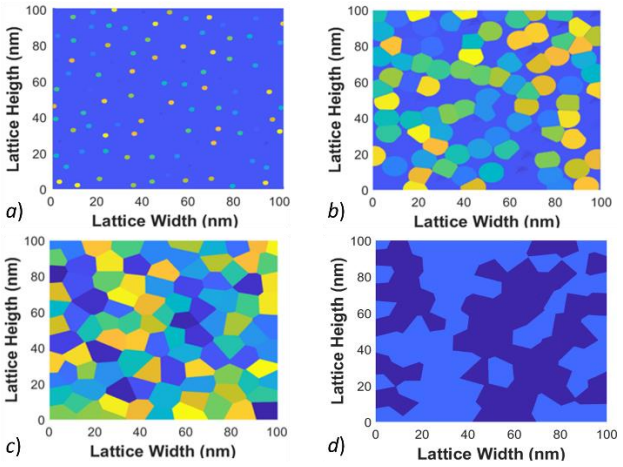

Fig. 1. Simulation stages of the irregular morphologies

III. Results

A. Domain size

With the number of initial growing points and the distance of separation between them we can control the domain size. The more initial growing points, the smaller domain size will be. Fig. 2 shows two morphologies, before assigning which material is each domain, for different number of initial points and domain sizes. The morphology in Fig. 2*a* was generated with 10 initial points and the average domain size is about 40 nm. Meanwhile, in Fig. 2*b* it was generated with 1000 initial points and its average domain size is about 4 nm.

B. Mixing ratio

In Fig. 3 is shown morphologies with different mixing ratio. They were generated with 1000 domain sizes, L_{min}=1nm, constant velocities and with cell size of 0.1 nm per side. The Fig. 3*a* has a similar morphology when it is compared with the characterized morphologies reported in [7] and [8].

C. Time consuming

Fig. 4 shows the simulation time as a function of cell size. From .1 nm to 2 nm of element size, the simulation time was less than one second. The minimum element size reached was 0.015 nm and it took approximately one hour to be simulated. Then the smaller the element of the cell, the matrix increases in size, as well as in resolution, therefore the more resolution the morphology has, the longer it will take to simulate.

IV. Conclusions

The proposed algorithm can simulate morphologies of the active layer that have been reported in the literature without a high time consuming. The domain size, the mixing ratio and the resolution can be controlled. If the resolution increase, then the simulation time increase.

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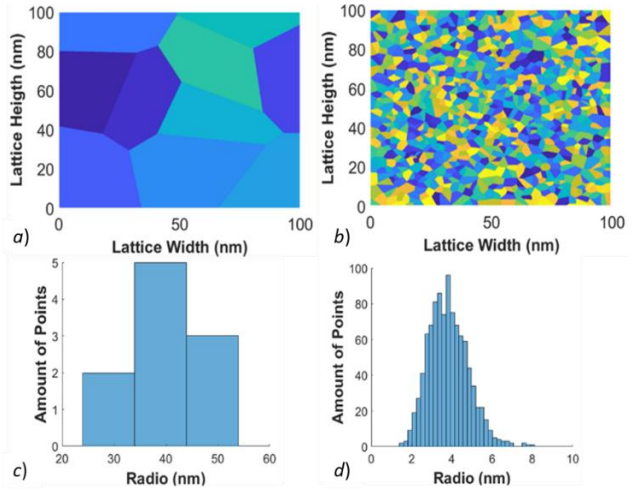

Fig. 2. Morphologies with different domain sizes.

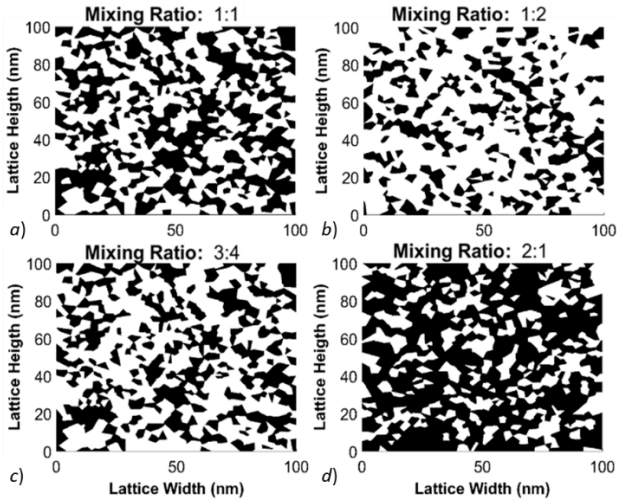

Fig. 3. Simulated irregular morphologies with different mixing ratio.

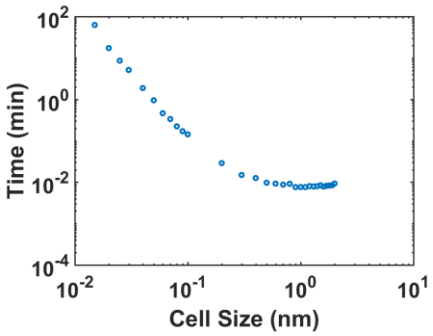

Fig. 4. Time consuming process as a function of cell size.

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