Intuition-Based Visual Modeling of Charge Transport Bottlenecks in Organic Photovoltaic Solar Cells

Amal Aboulhassan* KAUST
Olga Wodo† Iowa State University
Daniel Baum‡ Zuse Institute Berlin
Markus Hadwiger § KAUST
Baskar Ganapathysubramanian ¶ Iowa State University

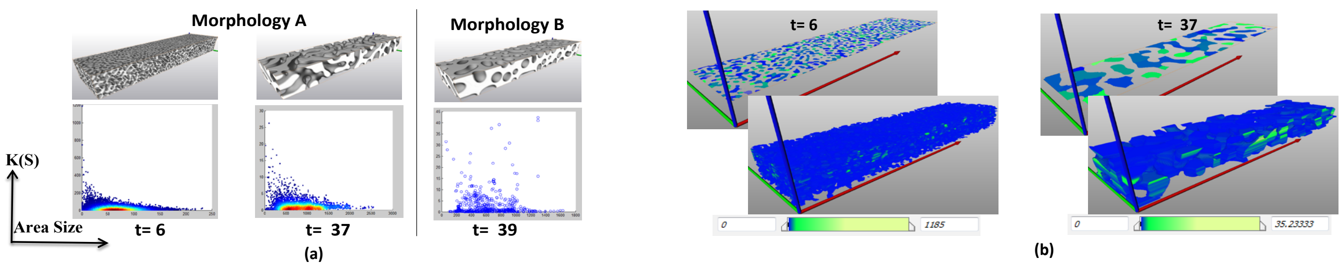

Figure 1: (a) Correlations between feature sizes in BHJ morphology and charge transport bottlenecks $K(S)$, for two different morphologies and at different simulation time steps. (b) Spatial analysis of bottlenecks through volume rendering, 1D transfer functions, and slices inside the volume to reveal cluttered parts. Each color-coded area is represented by one point in the scatter plot illustrated in (a).

Abstract

Current characterization methods for the bulk heterojunction (BHJ) morphology—the main material of recent organic photovoltaic solar cells—are limited to the analysis of global fabrication parameters. This reduces the efficiency of the BHJ design process, since it misses critical information about local performance indicators. Moreover, these approaches also do not help with intuitive analysis, which is widely adopted by the domain scientists. In this poster, we propose a novel application that fills this gap through visual characterization and exploration of one local performance indicator: *charge transport bottlenecks*. We propose a new intuition-based geometric model that correlates structural features with performance bottlenecks. Since our goal is to support the BHJ design, we assess the proposed model via its ability to extract correlations between features and bottlenecks. Moreover, we show that our approach can help reduce the BHJ analysis time from days to minutes.

1 Introduction and Domain Science Background

Organic photovoltaic (OPV) solar cells represent a new field of materials science which aims at providing a low cost, flexible alternative for harnessing solar energy. Since the OPV research is multidisciplinary, the community is developing intuition-based models to support unified analysis paradigms (e.g., [1, 5]). The underlying physical process is illustrated in Figure 2 (a). The intuition-based approximation model that is currently used [5] is summarized in Figure 2 (b). These intuition-based models are rooted in two main observations made by the domain scientists, as illustrated in Figures 2 (a) and (b). First, there is a relation between the geometric properties of charge paths and the physical parameters (examples can be found in the literature [1]). Second, there is a correlation between structural features and the shape of charge paths.

The traditionally used statistical tools [2, 5] lack means for local and spatial exploration. To handle this limitation, we propose a novel visual tool for the intuitive local characterization of the bulk heterojunction (BHJ) morphology—the main OPV material. In this poster, we focus on "charge transport bottlenecks." Scientists conceptually refer to bottlenecks in their characterizations, but still cannot fully analyze them due to the limitations mentioned above. In this poster, we illustrate our proposed geometry-based mapping of this physical indicator. Since a future goal of the project is BHJ fabrication, we assess our visual paradigm by the ability and time required for visualizing new correlations with structural features.

2 Bottleneck Model

Our bottleneck model is analogous to the familiar hour glass. If we slice an hour glass into planar cross-sectional areas, we will find that the bottlenecks exist at those positions where flux must pass through narrower areas. Accordingly, we consider our structural feature S to be a cross-sectional area across the route through the morphology. Then, we compute the charge path flux density gradient across each S. We start by computing the instantaneous rate of change of the flux density $j(s)$ along a given path s (Figure 2 (b)):

$$\kappa(s) = \frac{\mathrm{d}j(s)}{\mathrm{d}s}, \tag{1}$$

where $j(s)$ is the scalar flux density function on the path s, and its rate of change results in the *bottleneck coefficient* κ, characterizing the strength of a potential bottleneck along the path s. We also characterize a whole neighborhood (surface) with respect to there being a bottleneck by integrating over a cross-section as follows:

$$K(S) = \frac{1}{A}\int_S \|\nabla j\| \mathrm{d}S, \tag{2}$$

where S is the cross-sectional surface (discussed in the next subsection), and A is its area. $K(S) > 0$ indicates a bottleneck over S.

*e-mail: amal.aboulhassan@kaust.edu.sa
†e-mail:owodo@iastate.edu
‡e-mail:baum@zib.de
§e-mail:markus.hadwiger@kaust.edu.sa
¶e-mail:baskarg@iastate.edu

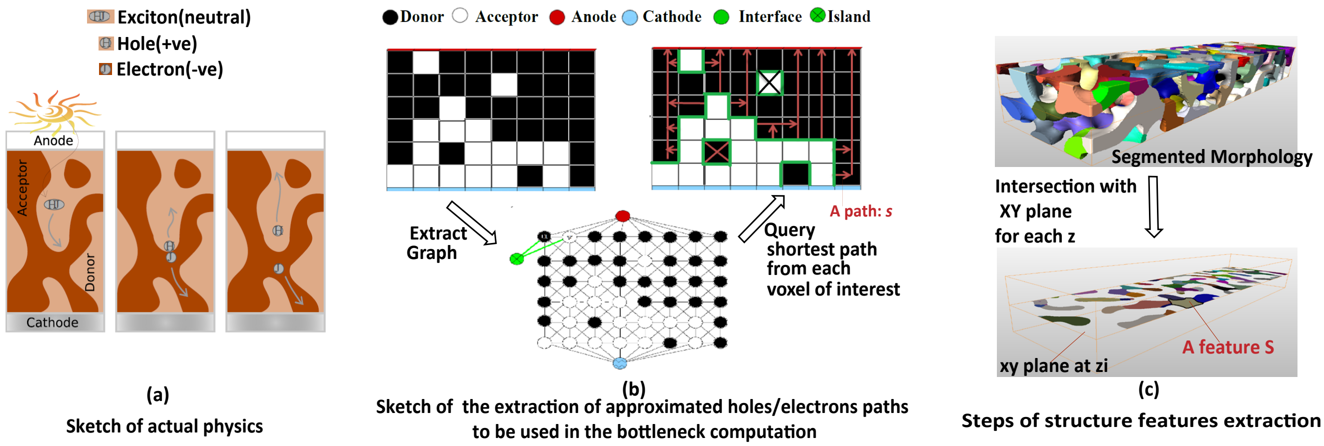

Figure 2: (a) the underlying physics of the photoelectric current process. The BHJ is a blend of two materials: *donor* and *acceptor*, which are separated by an *interface* and sandwiched between two electrodes (*anode* and *cathode*, respectively). The photoelectric current is generated in a sequence of stages: exciton generation, exciton diffusion, charge separation at the interface, charge transport, and charge collection at the electrodes. (b) the steps of extracting approximate charge paths from a BHJ volume [5]. Each BHJ volume is represented by a uniform grid. A graph is constructed from the volume, where each node represents one voxel and is labeled either 0 or 1(donor or acceptor, respectively). In the regions separating the donor and acceptor (the interface), the volume fraction changes from 0 to 1. By reconstructing the iso-contour corresponding to the iso-value 0.5, the interface can be identified. (c) the steps of extracting a structural feature S for the donor.

2.1 Extraction of Structural Features

We start by the following segmentation for each part of the domain (donor or acceptor). First, we compute a signed distance map, starting from all interface voxels. We use the Euclidean distance metric. If the distance map inside the regions that we are interested in has negative sign, we directly use this distance field. We then apply a watershed algorithm [4] and subsequently apply a persistence-based [3] merging step to create larger regions. To do so, we compare the scalar minima of two regions to be merged with the scalar value at the potential merge point. If the difference between one of the minima and the scalar value at the merge point is below a used-defined threshold, we merge the two regions. Otherwise, the regions are not merged. This way, we find a fair division of the morphology space. The boundaries of S are found through the intersection between the XY plane and each segment for each value of z as shown in Figure 2 (c). The size of S is defined by the voxels that belong to S mapped to the corresponding area in nm^2.

3 Visualization of Bottlenecks

We use “Morphology A” and “Morphology B,” fabricated using different lab conditions. Each time snapshot is of size 5.5 million voxels. The visualizations are implemented using the Avizo and Amira frameworks, Matlab, and GraSPI [5]. This study is done with domain scientists from the fields of physics and computational physics. We use scatter plots to summarize the correlation between size(S) and K(S) (Figure 1 (a)). Each point in the scatter plot denotes one S. Accordingly, the scatter plot is implicitly linked to the spatial data. The users have studied two time steps in morphology A. They also compared morphology A to morphology B. They can easily see correlations in A between the size and the bottlenecks (Figure 1 (a)). These correlations match the intuition since the strong bottlenecks cluster at small sizes and vice versa. This indicates the validity of our analysis. On the other hand, the correlations are not as clearly visible in B as in A. Here comes in one of the spatial analysis benefits where the result of B is attributed to the existence of more islands (defined in Figure 2 (b)) and appears in 3D in Figure 1 (a) (upper row). Moreover, it is possible to explore the exact locations of the high/low bottlenecks in A (Figure 1 (b)) for better insight into the design.

The morphology generation using GraSPI took 20 hours on a cluster with 160 CPUs, dual quad core nodes AMD Barcelona 2.2 GHz, and with 8 GB RAM. The time taken for generating charge paths is 15 minutes. The visualizations take a few seconds to generate (given that the computations are done offline). Accordingly, this analysis workflow eliminates hours of trial and error, and reduces the workflow to the order of minutes/seconds.

4 Future Work

The bottlenecks visualization introduced in the current poster is only a part of the full BHJ design process. Future aspects of analysis include: views less cluttered than volume rendering, interactive scatter plots, other intuitive models, connectivity analysis, and studying conflicting structure requirements among different charge path types. Furthermore, our paradigm could also be applicable to similar applications, such as vascular analysis and drug design.

Acknowledgements

This work was partially supported by King Abdullah University of Science and Technology (KAUST).

References

[1] A. Aboulhassan, R. Li, C. Knox, A. Amassian, M. Hadwiger. CrystalExplorer: An Interactive Knowledge-Assisted System for Visual Design of Solar Cell Crystal Structures. In Proceedings of Eurovis 2012 Short Papers; pp. 31-35, 2012.

[2] Gavin A Buxton and Nigel Clarke. Computer simulation of polymer solar cells. Modelling Simul. Mater. Sci. Eng. 15 (2007) 1326.

[3] H. Edelsbrunner, D. Letscher, and A. Zomorodian. Topological persistence and simplification. Discrete and Computational Geometry, 28(4):511533, 2002.

[4] M. Couprie, G. Bertrand. Topological gray-scale watershed transform. In Proc. of SPIE Vision Geometry V, volume 3168, (1997).

[5] Olga Wodo, Srikanta Tirthapura, Sumit Chaudhary, Baskar Ganapathysubramanian. A graph-based formulation for computational characterization of bulk HeteroJunction morphology, Organic Electronics, Volume 13, June 2012.