Morphology Effects in Dye Solar Cells

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Introduction

Solid state Dye Sensitized Solar Cells (ssDSCs) [1] are very promising photovoltaic devices, potentially stable, economical, and easy to integrate into existing architectural elements. A ssDSC is based on the fine intermixing between an electron- and a hole-conductor, often a thin nanostructured titanium dioxide layer onto which a monolayer of molecular organic dye (generally Ru-based) is chemisorbed, and an organic material (usually P3HT or Spiro-OmeTAD). The whole nanostructured composite, 2-3 μm thick, is sandwiched between two electrodes and encapsulated by a transparent sealant. Despite an intense investigation aimed at improving the macroscopic performance of these devices, many fundamental aspects of their behavior still need to be addressed. In particular charge diffusion through the nanostructured composite film must to be understood and modelled to drive the optimization of the device. The entire cell is usually modelled using drift-diffusion equations for both electrons and holes in an effective medium framework. By effective medium we mean that the real structure of the mesoporous materials are not explicitly taken into account in the model, and an effective material is used instead [2]. However, the real structure between electron- and hole-conductor materials is far more complex.

Discussion

Here we show that experimental structural data obtained from an electron tomography reconstruction of a ssDSC (figure 1, left) can be used as the input structure for charge transport simulations (figure 2). We then compare the results obtained using this experimental data to a similar cell structure treated with the effective medium approximation (figure 3). Charge transport in the device is computed using drift-diffusion equations coupled to Poisson equation for the electrostatic potential:

$$\nabla \cdot (\mu_{e(h)} n_{e(h)} \nabla \phi_{e(h)}) = (G - R). \qquad (1)$$

$$-\varepsilon_r \varepsilon_0 \triangle \varphi = \rho. \qquad (2)$$

In the previous equations $\mu_{e(h)}$ is the mobility, $n_{e(h)}$ the charge density and $\phi_{e(h)}$ the electrochemical potential for electrons (e) and holes (h). G is the generation term and R the recombination rate. ε_r the relative dielectric constant and ρ the local charge density. The total charge density depends on the local electron and hole densities and on trapped electrons at the interface between the two materials.

Conclusion

The model implemented is part of TiberCAD, a multiscale simulation tool [3] and includes all the components of the device consistently. This allows us to discuss the strengths and limitations of the widely-used effective medium model, but also to describe the transport properties of our ssDSC with unprecedented accuracy. In particular the effects of trap states and morphology to the current density and charge distribution can be explicitly addressed (figure 4).

References

[1] U. Bach et al., Nature **395**, 583-585 (1998).
[2] Alessio Gagliardi, Desire Gentilini and Aldo Di Carlo, Nature **116**, 23882-23889 (2012).
[3] M. Auf der Maur et al., IEEE Transaction on Electronic Devices **58**, 1425 (2011).

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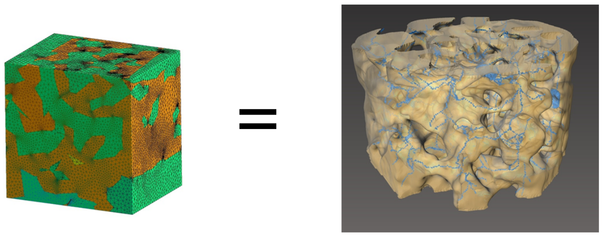

Fig. 1. *(color online) (Left) reconstruction of the real 3D blend by the mesher. (Right) experimental measurement of the TiO_2 structure.*

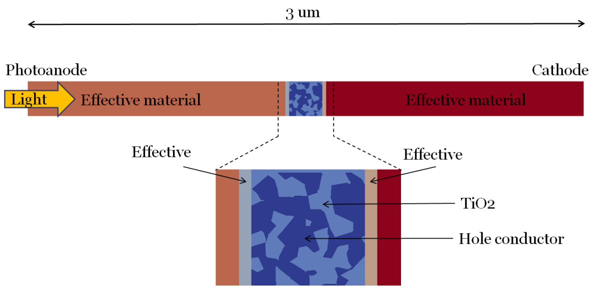

Fig. 2. *(color online) Emebedding of the real morphology (central region) within two regions modelled using the effective material for a 2D device. The mesh is divided in five parts, two regions close to the contacts (anode and cathode) with a less dense meshing, two buffering regions at the interface with a denser meshing but still using the effective material and a central region with a 2D slice of the real blend. The entire device is 3 μm long and the light comes from the left (anode) side. We assume periodic boundary conditions for the side boundaries of the cell.*

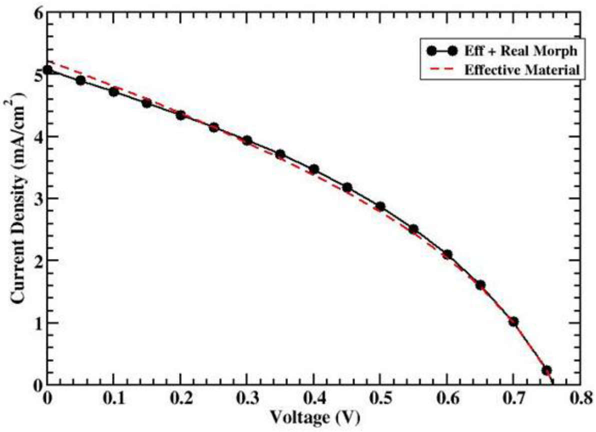

Fig. 3. *(color online) I-V characteristic of a ss-DSC modelled fully with an effective medium compared to an I-V including a central region with the real blend (see figure 2).*

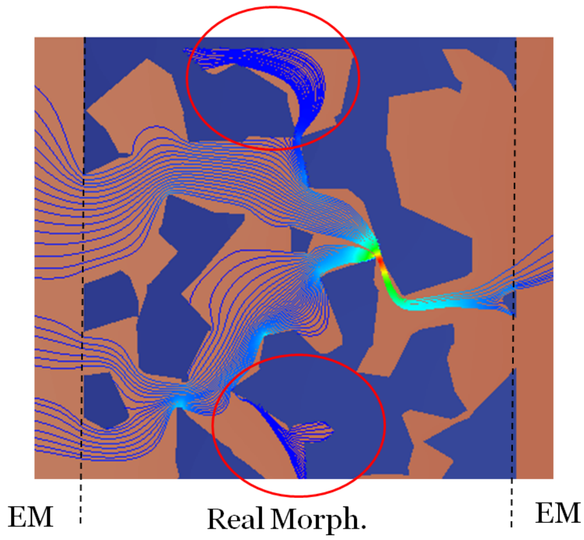

Fig. 4. *(color online) Hole current density inside the HTM (Real morphology region, in light red). The red circles underline regions where recombination currents occur. In the figure it is shown the propagation of holes also into the effective medium (EM) domains.*