Impact of Light Scattering on Efficiency Enhancement in Organic Solar Cells

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Summary: Further efficiency enhancements in organic solar cells require a deeper understanding of the charge generation and transport in the cell as well as the employment of advanced light trapping mechanisms. Both electronic and optical device models for organic solar cells have been developed already in the past. This paper, however, for the first time presents a simulation tool that combines a state of the art drift-diffusion electrical model with a complex optical model able to simulate wave propagation in thin film optics but also ray-based light propagation in incoherent layers and scalar scattering. The combination of the light-scattering algorithm and this drift-diffusion model leads to a coupled opto-electronic cell model [1] which represents a powerful design tool for cell characterization and optimization. This tool is then used to evaluate the gain of efficiency introduced by a light scattering interface made of a rough TCO in a bulk heterojunction (BHJ) solar cell. The results were found to be in good qualitative agreement with previously published experimental results [2].

1. Introduction

Modeling is an essential part in research of organic photovoltaic devices (OPVs) and speeds up their development. An accurate model can be used to gain further insight into device operation and for optimizing device performance. Difficulties to simulate state-of-the-art commercialized OPVs arise from the fact that these devices are not only made of an active thin-film layer stack, but also contain thick incoherent layers and scattering interfaces that enhance the light in-coupling and the light-trapping efficiency of the device.

In a first part of this paper we repeat the fundamentals of the microscopic charge transport model, previously implemented in the commercial simulation software SETFOS [1]. In the second part we introduce the macroscopic approach for optical and electrical modeling.

2. Electronic model

The key ingredients of the device model used in SETFOS were outlined in reference [3] and are reproduced below for clarity:

$$\frac{\partial E(x)}{\partial x} = \frac{e}{\varepsilon\varepsilon_0}\left(p(x) - n(x)\right) \tag{1}$$

$$J_e(x) = e\mu_e(n,T,E)\cdot n(x)\cdot E(x) - D(\mu,n,T,E)\cdot\frac{\partial n(x)}{\partial x} \tag{2}$$

$$\frac{\partial n(x)}{\partial t} + k_d(x)\cdot S(x) = \frac{1}{e}\frac{\partial J_e(x)}{\partial x} + r(x)\cdot p(x)\cdot n(x) \tag{3}$$

Here, n is the density of electrons, p the density of holes, E the electric field, S the exciton density, k_d the exciton dissociation rate into free charges and $r = \left(e/\varepsilon\varepsilon_0\right)\cdot\left(\mu_e + \mu_h\right)$ the Langevin recombination rate coefficient. Due to their disordered nature, polymers and small molecules have broadened HOMO and LUMO levels. In order to account for this effect in our charge transport model, we use a mobility model and a diffusion coefficient, that are both dependent on the electric field, the charge carriers concentration and the temperature as described in more detail in [4].

According to the Onsager Braun theory, the rate equation for excitons (S) contains two generation terms, and two decay terms. Excitons can either originate from the absorption of a photon ($\gamma.G_{opt}(x)$) (computed using the optical model described in the next part) or from the recombination of an electron and a hole ($r(x).n(x).p(x)$). Then excitons can either dissociate into free charge carriers ($k_d(x).S(x)$) or decay to the ground state ($k_f.S(x)$). The exciton continuity equation can then be written as the following:

$$\frac{\partial S(x)}{\partial t} = r(x)\cdot n(x)\cdot p(x) + \gamma \cdot G_{opt}(x) - \left(k_d(x) + k_f\right)\cdot S(x) \tag{4}$$

Finally, charge injection is assumed to be thermionic and affected by image charge recombination.

3. Optical models

The combination of multiple layers having thicknesses on different length scales with scattering layer interfaces make thin film organic solar cells complex optical devices.The optical model is able to simulate a stack with any sequence of incoherent and coherent layers including scattering interfaces between two incoherent layers.

Our optical model relies on a scalar light scattering algorithm for the simulation of thick incoherent layers coupled with a transfer matrix formalism for the simulation of coherent thin layer stacks. If the scattering behavior of an interface is well characterized, we can employ an innovative approach based on non-paraxial scalar scattering [5] to compute the light absorption from these complex multi-layer stacks. This original approach relies on the same physical assumptions as traditional one involving a ray-tracing tool: while the wave nature of light is considered in the thin film layer stack, only the intensity of light is considered in thick incoherent layers. However, the mathematical way to solve the problem does not rely on a Monte-Carlo algorithm, which is the case in ray-tracing simulations. This makes this approach much more computationally efficient. Moreover, this new model is fully integrated into the simulation software SETFOS which simplifies the workflow for comprehensive opto-electronic simulation of solar cells. The basic idea is to describe the light intensity distribution between 0° and 90° in each layer for forward and backward light propagation by a vector of dimension D, where D is the number of discrete angles. Propagation through the layers and reflection and transmission at the interfaces connect these flux vectors. In this approach, the effect of a scattering layer on the light propagation in the multilayer stack can be taken into account by introducing, instead of the scattering layer, a virtual interface that ‘summarizes’ the properties of the scattering layer in terms of reflection, transmission and absorption. We validated this optical model with EQE spectra of µc-Si solar cells deposited on textured and flat substrates [5].

4. Simulation of an OPV including a rough scattering interface

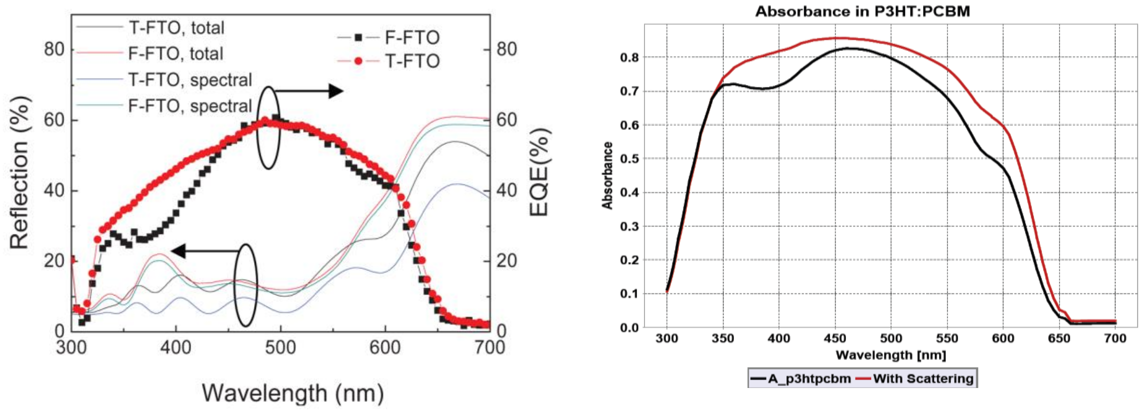
The combination of the light-scattering algorithm and this drift-diffusion model leads to a coupled opto-electronic cell model [1] which represents a powerful design tool for cell characterization and optimization. We show that this model can simulate the impact of a scattering interface on the overall performance of a BHJ organic solar cell.

To determine the amount of scattered light (haze), we employ the scalar scattering theory. It provides an analytical formula for the spectral dependence of the haze (H_T) in transmission, which is defined as the ratio between the diffusely scattered and the total light intensity given by [6]:

$$H_T = 1 - \exp\left[-\left(\frac{2\pi\sigma_{rms}\left|n_1 - n_2\right|c_T}{\lambda}\right)^2\right] \tag{5}$$

Here c_T represents a correction function, σ_{rms} the rms roughness of the interface λ the vacuum wavelength of the light and n the optical index. Then, we have assumed that the scatter part of the light follows a Lambertian law (i.e. a cos(θ) law). A more accurate description of the scattering function (not used in this work) can also be derived from AFM topography images.

In our simulation we find an increase in short-circuit current by 14% and an increase of the power conversion efficiency by 13 %. These results are in good qualitative agreement with recently published experimental results with BHJ cells with a scattering transparent conductive oxide electrode interface [2], see Figures 1 and 2 below.


(a)

(b)

Figure1 : Performance comparison of BHJ organic solar cell with flat fluor-tin oxide (F-FTO) electrode interface (black) and textured/scattering FTO (T-FTO) electrode (red): a) measured spectral EQE from [2], b) calculated spectral absorbance in the active layer.

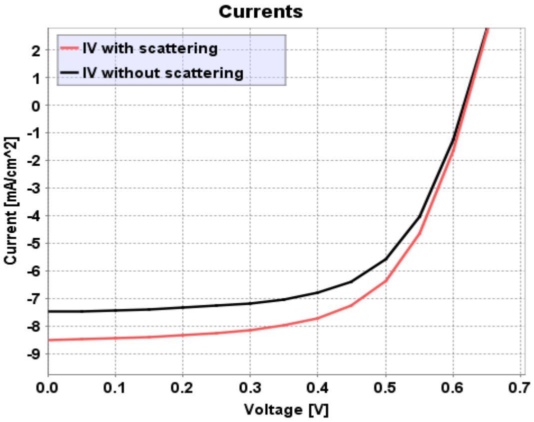


Figure 2 : Calculated current-voltage curve of a BHJ organic solar cell including a scattering FTO electrode (red line) or only flat interfaces (black line)

5. Conclusion

In this paper an opto-electrical model for designing OPVs is presented. The electrical model accounts for the microscopic charge transport in OPVs and the optical model accounts for both wave propagation in thin films layer and ray-based light propagation and scalar scattering in incoherent layers. This model was then used to simulate a BHJ solar cell containing a rough transparent electrode. It is found that the light scattering, induced by the rough interface, leads to a significant increase of the OPV performance in good agreement with previously published results.

References:

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