Numerical Analysis and Optimization of PEDOT:PSS/Si Nanowire Hybrid Solar Cells

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***Abstract*—In this paper, a numerical program for simulating the organic/inorganic hybrid solar cells is developed first by including the tail/interfacial states for carrier transport of the organic materials. Then a typical structure of the PEDOT:PSS/Si nanowire hybrid solar cell is simulated and compared with experimental results. Finally, an efficiency up to 14% is obtained after the optimization.**

***Keywords*—Hybrid solar cells, PEDOT:PSS, silicon nanowire, simulation**

I. Introduction

Due to the increasing demand of the electrical energy and the shortage of fossil fuels, solar energy has drawn a strong attention as an alternative energy source. Among all the solar cells, organic/inorganic hybrid solar cells has the advantages of potential low-cost, easy fabrication and the flexibility which leads great interest in studying the organic/inorganic hybrid solar cells. Plenty of the experimental researches about the organic/inorganic solar cells are published, but only few numerical analyses of such solar cells were studied owing to the ambiguous carrier transport properties of the organic materials. In this paper, poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS) and silicon (Si) are used as the organic and inorganic material, respectively. Here, we include a new model to present the carrier transport property of the PEDOT:PSS.

II. Simulation Model and Methodology

The simulation model of PEDOT:PSS/silicon nanowire (SiNW) hybrid solar cells and the structural dimensions are shown in Fig. 1. In this model, the organic material, PEDOT:PSS has the advantages of transparency, high conductivity, and high hole mobility compared with other organic materials, while the crystalline silicon is often chosen as the absorber due to the relative low-cost and good efficiency.

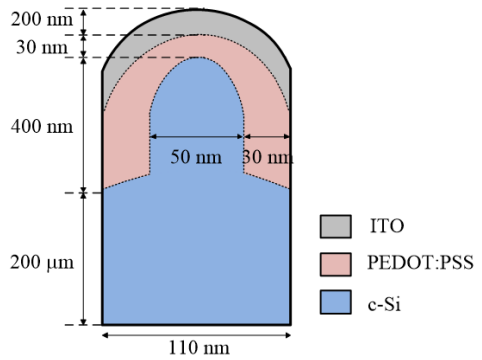

Fig. 1: Simulation model of PEDOT:PSS/SiNW hybrid solar cells

The absorption coefficient of both materials is worth of notice that the PEDOT:PSS has stronger absorption in the long wavelength range than the silicon does [1, 2]. This is owing to the existence of tail states in the PEDOT:PSS that not only allowing the wavelengths with photon energy smaller than the bandgap energy to be absorbed, but also providing the carriers new path ways to hop around those tail states that are located in between the lowest unoccupied molecular orbitals (LUMO) and the highest occupied molecular orbitals (HOMO). Hence, the distribution of tails states in PEDOT:PSS is critical to be taken into account when considering the carrier transport property of PEDOT:PSS. Here, we propose a Gaussian distribution function (1) of tail states to present the carrier transport in PEDOT:PSS.

$$N_{tail,dos}(E) = N_t \frac{1}{\sigma\sqrt{2\pi}}\, exp\left[-\frac{(E-E_t)^2}{2\sigma^2}\right], \qquad (1)$$

where E_t is difference between the center of the distribution and the band edge (LUMO or HOMO), σ is one half of the full width at half maximum (FWHM) of the distribution and N_t is the total number of density of tail states calculated by

$$N_t = \int_{-\infty}^{\infty} N_{tail,dos}(E)\, dE. \qquad (2)$$

The tail states will be added around the LUMO and HOMO for electrons and holes to transport, respectively. The optical field is calculated by applying 2D-FDTD method. Next, the performance of PEDOT:PSS/SiNW hybrid solar cells is obtained by using the Poissons and drift-diffusion solver [3].

III. Results And Discussion

Fig. 2 is the J-V curve of simulation results based on the structure illustrated in Fig. 1, and the simulation parameters are verified by fitting the experimental J-V curves of the planar PEDOT:PSS/Si hybrid solar cell shown in Fig. 3. It's obvious to see that the performance of V_{oc} and the fill factor (FF) are not very good if we compare the result with the conventional silicon-based solar cells. Therefore, we analyze the loss mechanisms in the PEDOT:PSS/SiNW hybrid solar

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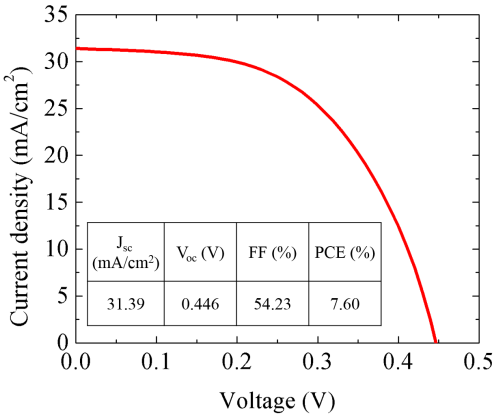

Fig. 2: The J-V curve of simulated PEDOT:PSS/SiNW hybrid solar cells.

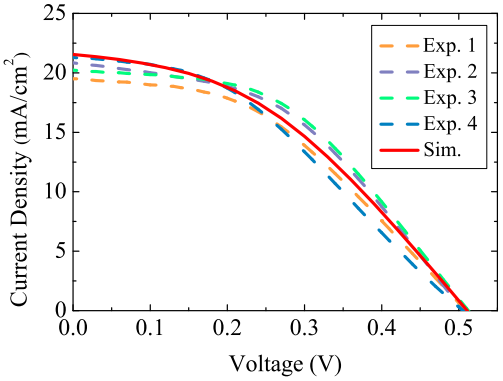

Fig. 3: The J-V curve of experimental and simulated planar PEDOT:PSS/Si hybrid solar cells.

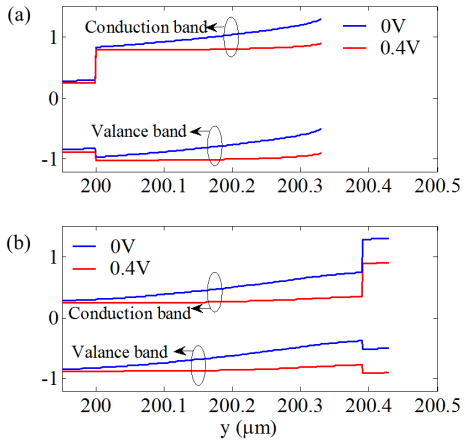

Fig. 4: The band diagram along y-axis for applied voltage V = 0 (blue solid line) and 0.4 V (red solid line) at (a) x = 0 and (b) x = 50 nm.

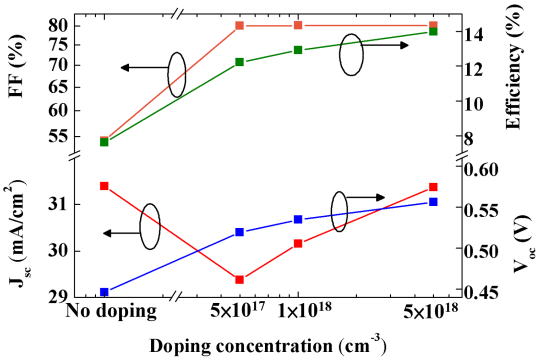

Fig. 5: The J-V curve of PEDOT:PSS/SiNW hybrid solar cells under the different conditions of doping concentration.

cell at different applied voltages. It's found that the change of applied voltage has great effect on the silicon interface region, and the main reason is due to the small depletion field at the interface illustrated in Fig. 4.

Hence, we further optimize the structure by adding a p-type layer to create a stronger depletion field at the interface, and the results are shown in Fig. 5. With an extra p-type layer adding at the interface, it's found that the FF has great improvement, leading to a better efficiency. The highest efficiency 13.97% is obtained with p-type doping concentration = 5×10^{18} cm^{-3}. Except improving the FF, it's also found that the non-radiative recombination at the PEDOT:PSS/Si interface also plays an important role. However, to improve it, we will need some new idea of passivation technology.

IV. Conclusion

In this paper, we propose a model for simulating the organic/inorganic hybrid solar cells. After analyzing the loss mechanism, it's found that the key issue is the small depletion field that results in small V_{oc} and FF. Therefore, we further aim at improving the depletion field at the interface by adding a p-type layer at the interface, and an efficiency up to 14% can be obtained.

V. Acknowledgments

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