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Relation between Spatial Distribution of Plasmonic Nanoparticles and Photovoltaic Parameters in Organic Bulk Heterojunction Solar Cells

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Abstract- Despite interesting physical flexibility and low-cost fabrication process, OSCs has low efficiency due to the low light absorption. Due to the unique electro-optical properties of plasmonic nanoparticles (NPs) such as high absorption and light concentration, the metallic NPs opened a potential application for enhancement of characteristics parameters of OSCs. Implementing plasmonic NPs in host layer of OSC causes changing in electronic properties such as light absorption, conductivity, diffusion length. Spatial distribution of plasmonic NPs directly affect the absorption and charge carrier transportation through active layer. In this paper, we perform the simulation analysis for investigation of metallic NPs spatial location in near anode, middle and near cathode, on characteristics parameters of OSCs via the drift-diffusion model. Our results show that spatial redistribution of NPs can be boost both short circuit current and open circuit voltage and simultaneously, power conversion efficiency. The simulation results show that best efficiency achieves in spatial distribution of NPs in middle of active region that are in good agreement with published reports.

Keywords: Organic Solar Cells, Plasmonic Nanoparticles, Efficiency

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1. Introduction

In recent years, many researches are done to increase the efficiency of organic bulk heterojunction organic solar cells (BHJ OSC), as well as flexible, lightweight, and low-cost manufacturing techniques [1-2]. Low light absorption causes charge carrier recombination losses and low fill factor, therefore, researches are done to finding solutions to increase light absorption through active region of BHJ OSCs. Due to the unique electro-optical properties of plasmonic nanoparticles (NPs) such as high absorption, the metallic NPs have been introduced a potential application for enhancement of characteristics parameters of OSCs. Two types of plasmonic resonances NPs can be used for enhancing light absorption: surface plasmonic resonances (SPRs) [2] and localized plasmonic resonances (LPRs) [3]. Implementing plasmonic NPs in the host layer of OSC causes changes in electronic properties such as light absorption, conductivity, and diffusion length. Spatial distribution of NPs in host materials near anode, center, and near cathode has different effects on spatial distribution for excitons [4].

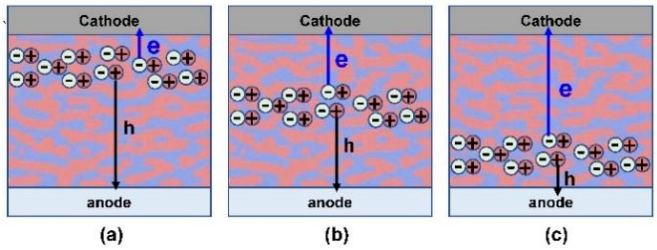

Fig. 1: Schematic diagrams of the plasmonic NPs OSCs with generated charge carriers and the spatial location at (a) near the anode, (b) middle, and (c) near the cathode.

The electrical behavior of OSCs can be predicted by solving a self-consistent drift-diffusion numerical models, wherein this study, by solving self-consistent drift-diffusion and Poisson equation via Finite Element Method (FEM) and considering the boundary condition, exciton density, short circuit current (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), efficiency (η) and J-V characteristics have been calculated. Our results show that spatial redistribution of NPs can boost both short circuit current and open-circuit voltage and simultaneously, power conversion efficiency.

2. Models and Methods

Recombination in the active region consists of different models such as bimolecular or Langevin recombination, Shockley-Read-Hall (SRH) recombination, or trap assisted and geminate recombination, that we have been taken into account in numerical simulations. In our study, we solve these equations via FEM by applying the boundary conditions and 100 nm active layer thickness. Finally, by calculating the charge continuity equations, it is possible to calculate J_{sc}, V_{oc}, FF, η, and J-V characteristics.

3. Results and Discussion

In our simulation, Ag metallic nanoparticles were selected as plasmonic NPs (Fig. 1). Fig. 2 (a) shows the charge carriers generation rate by implementing Ag NPs in the active region. Inserting NPs in the active region creates extra charge carrier generation. As it was shown, inserting NPs in the middle of the active region, maximizes charge carrier generation. The increasing of carrier generation leads to higher concentrations n and p. The density of excitons, S, also increases for larger carrier generation process Fig.2 (b). We observe the same distribution of the S(x) curve with generation rate which is a consequence of NPs behavior.

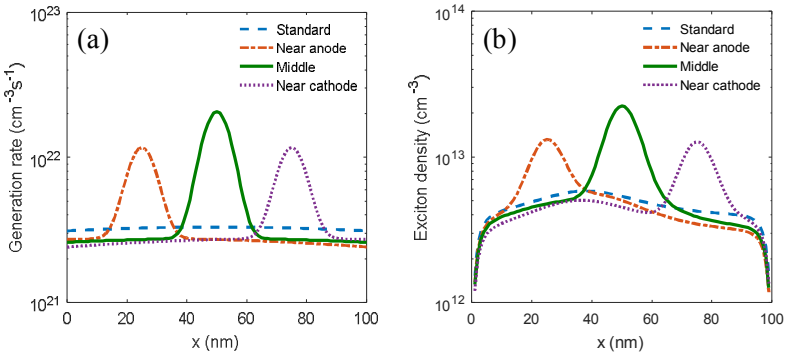

Fig. 3: (Color online) (a) Charge carrier generation rate in without NPs and in different spatial location of NPs (b) spatial distribution of excitons density with and without NPs.

Our calculations clearly illustrate that the density S increases in NPs spatial location. Inserting NPs in the middle of the active region leads to extra charge carrier generation and also, controlling the photocarrier transport path. It is well known that increasing exciton density leads to an increase in cell efficiency. J-V curve helps to understand the detailed influences of inserting NPs in the active region of OSC. J-V characteristics of the proposed device shown in Fig. 3. Inserting NPs in the middle of the cell boosts J_{sc} and V_{oc}.

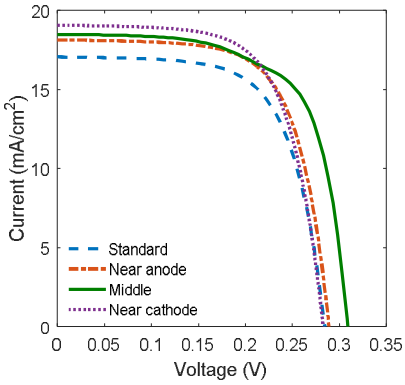

Fig. 3: (Color online) J-V characteristics in three different spatial location of NPs.

In P3HT:PCBM BHJ OSC, electron mobility lower than holes, so, in the case of near cathode condition, J_{sc} slightly higher than the middle and near anode that, because of collecting rapidly electrons by the cathode. From the simulation results in Table I, the middle case has higher V_{oc} and higher FF and consequently, higher power efficiency.

Table I. Electrical parameters for without NPs and plasmonic OSC with different NPs spatial distribution.

NPs position	J_{sc} (mA/cm^2)	V_{oc} (V)	FF	η (%)
Standard	17.10	0.28	0.61	2.95
Near anode	18.13	0.29	0.62	3.28
Middle	18.50	0.31	0.64	3.64
Near cathode	19.06	0.28	0.62	3.37

It was shown the dense exciton generation around plasmonic nanostructures provides a flexible and integrated way to both increase J_{sc} and simultaneously boost V_{oc} and FF [4] and our results are in good agreement with previously published data [4]. As shown in Fig. 2 (b) NPs produce non-uniformly distributed excitons that lead to manipulating transport paths of charge carriers to equalize the transport time of electrons and holes and reduce space charge region. Our results rival that spatial redistribution of NPs in the middle causes higher charge carrier densities and higher exciton generation and leads to boost both short circuit current and open-circuit voltage and power conversion efficiency, respectively.

4. Conclusion

In conclusion, the plasmonic NPs OSCs with generated charge carriers and the spatial location near the anode, the middle, and near the cathode have simulated via drift-diffusion equations by considering recombination processes and plasmonic NPs absorption. In our simulation, Ag metallic nanoparticles were selected as plasmonic NPs. Placing NPs produce in middle of active region lead to manipulating transport paths of charge carriers to equalize the transport time of electrons and holes and lead to efficiency enhancement. Our results show that spatial redistribution of NPs in the middle of the active region can boost both short circuit current and open-circuit voltage and simultaneously, power conversion efficiency.

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