The Effect of Plasmonic Nanoparticles and the Thickness of Anode Interface Layer on the Efficiency Enhancement of Organic Solar Cells

Neda Ahmadi (ahmadiphysic@gmail.com)
Islamic Azad University Garmsar Branch https://orcid.org/0000-0002-6168-0121

Research Article

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The effect of plasmonic nanoparticles and the thickness of anode interface layer on the efficiency enhancement of organic solar cells

Neda Ahmadi *

Department of Basic Sciences, Garmsar Branch, Islamic Azad University, Garmsar, Iran

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Abstract

We investigate the effect of nanoparticles (NPs) position on the optical parameters of organic solar cells (OSCs). We change the position of NPs inside the anode interface layer (AIL) and active layer and study the role of NPs position in light transmission, power absorption, short-circuit current density (Jsc), and maximum generation rate. We also use silver (Ag) nanoparticles inside the anode interface layer and investigate the optical parameters. Moreover, we study the role of AIL thickness in light transmission and power absorption. We use finite-different time-domain (FDTD) method for all simulations. This study can be useful for new perspectives and light management in organic solar cells.

Keywords: Organic solar cells, Plasmonic nanoparticles, Transmission, Generation rate, Anode interface layer, Power absorption.

*E-mail: n.ahmadi@srbiau.ac.ir, ahmadiphysic@gmail.com
1 Introduction

Photovoltaic technologies are the best solution for climate changes in order to using renewable and sustainable energy. For these reasons extensive effort have been concentrated on developing new generations of this technology such as Organic solar cells, Quantum dot solar cells, Perovskite solar cells [1, 2, 3, 4] etc. Organic solar cells are cheaper than current silicon-based technology and the process of manufacturing of them is easier than silicon-based solar cells. They also have the salient features such as light weight, flexibility and tunable transparency [5, 6, 7] etc., even though, they have low power conversion efficiency.

Recent OSCs have over 10% power conversion efficiency (PCE) based on single-junction devices. Single-junction terrestrial OSCs have reached an efficiency of 11.2 ± 0.3 under the global spectrum (1000 w/m²) at 25° c [8]. On the other hand tandem OSCs have achieved 10.6% PCE under standard test conditions [9]. These days, theoretical studies have shown that PCEs of tandem OSCs can achieve 15-20% by optimizing the active layer properties and device architectures [10, 11].

One of the promising way to increase the efficiency enhancement of solar cells is plasmonic nanoparticles [15, 16, 17]. For example in the previous work we investigated the effect of plasmonic nanoparticles on efficiency enhancement of thin film silicon solar cells [18]. We found that using metallic nanoparticles improve the efficiency of silicon-based solar cells because NPs create highly concentrated on near-field, increasing pathlength due to far-field scattering and wave guide coupling [11].

In previous studies we worked on optical properties of nanomaterials [12, 13, 14]. In this work we study the effect of plasmonic nanoparticles on OSCs. We have used Poly (3,4-ethylenedioxytiophene): poly (styrene sulfonate) (PEDOT:PSS) as an anode interface layer (AIL) and Poly (3-hexylthiophene) (P3HT) and [6,6]-Phenyl-C61-butyric acid methyl ester (PCBM) (P3HT:PCBM) as an active layer. Nano particles are located at these layers and investigate the optical parameters. We have also optimized AIL thicknesses and study the effect of variation of thickness on power absorption and light transmission.

2 Method and formalism

In this article we use finite difference time domain (FDTD ) method solving Maxwell’s equations for our simulation. We investigated the effect of plasmonic nanoparticles on the efficiency of typical OSC with a photoactive layer of bilayer planar heterojunction which is sandwiched between two electrode.

The sunlight ranging is from 300 to 750 nm. We use two kind of nanoparticles Ag and Au and compare the effects of them. The radius of these NPs is 30 nm and complex index (n,k) of Ag and Au were fitted from reference[19].

We use Al; a metal with low work function (WF), with dimensions: X=2, Y=2, Z=0.5 μm as cathode which was taken from reference [20] and zinc oxide (Zno) as cathode interface layer (CIL) with thickness 0.07 μm. Zinc oxide (Zno) is an inorganic n-type semiconductor is one of the best materials for metal oxide cathode interface layer because it has low cost, easy synthesis, non-toxic properties [21] etc., and this material was fitted from reference[22].
We use Indium tin oxide (ITO) as Anode was taken from reference [23] with thickness \(Z=0.178 \mu m\).

Active layer is Poly (3-hexylthiophene) (P3HT) and [6,6]-PhenylC61-Butyric acid methyl ester (PCBM) (P3HT:PCBM) were fitted from [24, 25]. The dimensions of active layer are: \(X=2, Y=2\) and \(Z=0.193 \mu m\).

Poly (3,4-ethylenedioxythiophene): poly (styrene sulfonate) (PEDOT:PSS) is used as an anode interface layer to modify the ITO electrode and was fitted from [24].

3 Result and Discussion

3.1 Gold (Au) NPs located inside Anode interface layer

Light trapping in OGCs is a promising way to increase PCE. There are several techniques for light trapping in OSCs including of periodic nanostructures [26, 27, 28], diffraction grating [29, 30], metallic nanoparticles [31] and using grating and metallic nanoparticles [32].

Metallic nanoparticles can enhance the absorption of light due to two mechanisms. One of them is the increasing of forward scattering cross section and the second is a near field enhancement [33]. In this work we investigate the effect of NPs position on OSCs. Previous experimentally literatures have shown that metal NPs position is one of the most important factor for efficiency enhancement of OSCs [10, 34, 17]. The experimental results show that metal NPs are usually placed inside the AIL [35]. There are different fabrication methods such as electrodiposition [36], thin film evaporation [37] and chemical synthesis [39] which used to combine metal NPs into OSCs.

Table 1 shows short circuit current density; \(J_{sc}\), current and generation rate for different position of Au NPs with diameter 30nm. It is clear that in this device structure we have optical parameters enhancement compare with previous works [38].

| OSC type                           | \(J_{sc}\) \(\frac{mA}{cm^2}\) | Current A \(A\) | Maximum generation rate \(\frac{1}{m^3} \cdot \frac{1}{s}\) |
|-----------------------------------|-------------------------------|----------------|-----------------------------------------------|
| NPs are located at the active layer | 19.107                       | 7.002 \(\times 10^{-11}\) | 3.577 \(\times 10^{28}\)                     |
| NPs are located at the highest part of AIL | 19.197                       | 7.036 \(\times 10^{-11}\) | 1.662 \(\times 10^{29}\)                     |
| NPs are located at the middle part of AIL | 19.243                       | 7.052 \(\times 10^{-11}\) | 1.986 \(\times 10^{29}\)                     |
| NPs are located at the lowest part of AIL | 19.665                       | 7.207 \(\times 10^{-11}\) | 2.361 \(\times 10^{29}\)                     |
| Standard OSC                      | 19.007                       | 6.966 \(\times 10^{-11}\) | 6.531 \(\times 10^{27}\)                     |

Table 1: OPV parameters for standard OSC and plasmonic OSC with different positions of NPs.

The generation rate is according to the following equation,

\[ G \sim P = \frac{1}{2} \varepsilon'' \omega |E|^2, \]

where \(G\) is the exciton generation rate, \(P\) is the electromagnetic energy dissipation rate, \(\varepsilon''\) is the imaginary part of complex permittivity, \(\omega\) is the angular frequency of electromagnetic wave and \(E\) is the local electric field [40].
Fig. 1 shows the schematic drawing of standard polymer heterojunction solar cell. We have used Au nanospheres inside the active layer and AIL and have investigated the effect of the position of nanoparticles on efficiency enhancement of OSC with 3D FDTD simulation.

In Fig. 2 we can see the transmission spectrum of a standard OSC (without nanoparticles) and OSC with nanoparticles in different positions. We use Au NPs with diameter 30nm inside the AIL with thickness 140 nm. It seems that OSC with NPs are located at middle and highest part of AIL has maximum transmission.

Fig. 3 compares the power absorption of OSC in different modes. As can be seen, power absorption of OSC when the NPs are located in the lowest part of AIL for long wavelength; 635-750 nm, is greater than other.

3.2 Silver (Ag) NPs located inside Anode interface layer

Gold, silver, copper and aluminum are used in the photovoltaic devices as metallic nanoparticles because these metals can strongly interact with the sunlight [41]. Here we use Ag NPs with radius 30 nm inside the middle of AIL and compare the transmission and power absorption spectrum with Au NPs with 30nm radius. Fig. 4(a) illustrates the transmission spectrum of OSC with Au and Ag NPs. As we can see, approximately there is no difference between the transmission spectrum of OSC when Ag and Au NPs are located at AIL. In Fig 4 (b) it is clear that the power absorption spectrum of OSC for Au NPs is more than Ag for the middle range of wavelength spectrum and these results agree with previous works [41].

3.3 Variation of AIL thickness

In this section we have changed the AIL thickness of standard OSC from 140 nm to 50 nm and have investigated the effect of thickness on light transmission, power absorption and other device parameters. As shown in Fig. 5(a) we can see the transmission spectrum for different thickness of AIL. It seems that the increase of thickness decreases the transmission for the wavelength between 300-630nm and for wavelength more than 630nm the rise of thickness causes the increase of light transmission. In Fig 5 (b) we can see the variations of power absorption in term of wavelength. The enhanced device parameters were obtained for different AIL thickness as shown in table 2.

| AIL thickness | Jsc mA/cm² | Current A | Maximum generation rate $\frac{1}{m^3}$s⁻¹ |
|---------------|------------|-----------|------------------------------------------|
| 140 nm        | 18.951     | 6.945 x 10⁻¹¹ | 6.530 x 10²⁷                      |
| 100nm         | 18.384     | 6.737 x 10⁻¹¹ | 6.544 x 10²⁷                      |
| 50nm          | 17.641     | 6.465 x 10⁻¹¹ | 6.809 x 10²⁷                      |

Table 2: OPV parameters with variation of AIL thickness.
4 Conclusions

In this work we investigated the role of NPs position in the optical parameters of OSC and found that the position of NPs in the AIL and active layer is an important factor which modifies the optical parameters of OSC. We also compared the light transmission and power absorption spectrum for Au and Ag nanoparticles when they are located in the middle of AIL and found that the absorption spectrum of Au NPs is greater than Ag for the visible wavelength thus they are appropriate for the visible spectrum. This study opens new aspect in OSCs for light management.

5 Declarations

5.1 Funding
Not applicable

5.2 Conflicts of interest/Competing interests
Not applicable

5.3 Availability of data and material
Available

5.4 Code availability
Not applicable

5.5 Authors’ contributions
Not applicable

5.6 Ethics approval
We believe that this manuscript is appropriate for publication by Plasmonics journal because it creates a paradigm for future studies. This manuscript has not been published and is not under consideration for publication elsewhere.

5.7 Consent to participate
Not applicable

5.8 Consent for publication
I give my consent for the publication of this manuscript which includes tables and figures in the Plasmonics journal.
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Figure 1: Schematic drawing of organic solar cell.

Figure 2: Light transmission of organic solar cell with Au nanoparticles embedded in different positions of PEDOT:PSS and standard organic solar cell.

Figure 3: Power absorption of organic solar cell with Au nanoparticles embedded in different positions of PEDOT:PSS and standard organic solar cell.

Figure 4: (a) Light transmission (b) Power absorption of organic solar cell with Au and Ag nanoparticles embedded in the middle part of PEDOT:PSS.

Figure 5: (a) Light transmission (b) Power absorption of organic solar cell with different thickness of PEDOT:PSS.
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