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Plasmonic Organic Solar Cell and Its Absorption Enhancement Analysis Using Cylindrical Ag Nano-Particle Model based on Finite Difference Time Domain (FDTD)

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Abstract: We report the plasmon-assisted photocurrent enhancement in Ag nanoparticles (NPs)-embedded PEDOT:PSS/P3HT:PCBM organic solar cells, and theoretically investigate the causes of the improved optical absorption based on a cylindrical Ag-NPs model which is simulated with a finite difference time domain (FDTD) method. The proposed cylindrical Ag-NPs model is able to explain the optical absorption enhancement by the localized surface plasmon resonance (LSPR) modes, and to provide a further understanding of Ag-NPs shape parameters which play an important role to determine the broadband absorption phenomena in plasmonic organic solar cells.

OCIS codes: (160.4236) Nanomaterials; (240.6680) Surface Plasmons; (160.4890) Organic materials

1. Introduction

Discontinuous metal thin film prepared by an electron-beam deposition technique can provide an easy way to induce the localized surface plasmon resonance (LSPR) effect which is originated from collective electron charge oscillations in the metallic nanoparticles or cluster surfaces embedded in thin film organic solar cells. Thus, such metallic inclusions in a form of NPs or nanoclusters have been used as a device element for constructing an efficient solar cell while overcoming the weak absorbance of sun light in the active layer [1]-[2].

In this letter, we fabricated the plasmonic enhanced P3HT:PCBM bulk heterojunction solar cells using a simple electron-beam deposition technique, and their improved photocurrent was analyzed by introducing a cylindrical NPs model using Finite Difference Time Domain (FDTD). The two dimensional Ag-NPs model was useful to understand the spatial distributions of enhanced electromagnetic field density depending on the wavelengths, and the Ag-NPs shape parameters in the dispersive BHJ dielectric material.

2. Experiment and Results

Electron-beam deposition of Ag metal on ITO was performed with a deposition rate of 0.1 Å/sec. A buffer layer of poly(ethylenedioxythiophene) doped with poly(styrenesulfonate) (PEDOT:PSS) was spin-coated using an aqueous solution (Baytron PVP Al 4083) onto Ag NPs/ITO substrate, followed by annealing at 120 °C for 15 min under air environment. Then, the active material containing P3HT and PCBM with 1:1 weight ratio dissolved in 1,2-dichlorobenzene were spin-casted onto PEDOT:PSS to be ~140 nm thick, followed by annealing process at 140 °C for 5 min in a glove box. Finally, the LiF/Al cathode was made using a thermal evaporation technique (Fig. 1(a)). We have experimentally observed that the solar cell efficiency was increased as a function of silver thickness and at a thickness of 5 nm, a 60 % increase of the photo-conversion efficiency was achieved as shown in Fig. 1(b).

We have simulated a shape of NPs having a truncated Ag island spheroid which is cut about one third from the bottom. But it was not able to explain the photocurrent enhancement because LSPRs modes are tightly localized in the vicinity of the Ag-NPs within the PEDOT:PSS and ITO layers, resulting a very limited contribution to the enhancement of the optical absorbance in our case. Therefore, we have introduced a cylindrical Ag-NPs model from the AFM estimation in Fig. 2(a). This model was able to elucidate the causes of the absorption enhancement due to LSPRs by simplifying the shape of Ag-NPs to be two-dimensionally distributed cylindrical NPs. The thickness of the PEDOT:PSS layer was experimentally estimated to be ~20 nm thick, and that of Ag-NPs was ranging from a couple of nm to tens of nm showing a highly inhomogeneous surface. The small sizes of Ag-NPs didn't contribute to the light absorption enhancement even if their LSPRs clearly existed. Therefore, only large sizes of Ag-NPs close to ~20 nm thick were considered for the device model. The average sizes of the Ag-NPs in AFM investigation (Fig. 2(a)) were estimated to be ~60 nm wide and ~20 nm height. Finally, these parameters were used to make an uniformly dispersed cylindrical Ag-NPs onto ITO, and mixed with PEDOT:PSS dielectric as shown in Fig. 2(b)-(d).

Fig. 3(a)-(c) shows the excitation of LRPRs in the vicinity of Ag-NPs, creating strong electromagnetic fields and evanescently propagating waves that could enhance the light absorption, and thus, the photocurrent of the organic solar cells. Such strong electric fields are occurred at the corners of the cylindrical Ag-NPs that are tightly confined but evanescently spreading into neighbors. Examining the field patterns at three wavelengths (415 nm, 536 nm, and 625 nm) at both interfaces identifies two important factors for the optical absorption enhancement process. First, all the optical wavelengths do not participate in the increase of the optical absorbance even if exhibiting their own strong electric field enhancement. Second, the strength and frequency of LSPRs not only depend on NPs size, and distributions, but also become sensitive to changes in surrounding dielectric environment. In order to investigate the effects of Ag-NPs distributions, a 2D-cylindrical model has been simulated as shown in Fig. 3(d). The optical absorbance increases significantly at wavelengths of 440 nm ~ 650 nm when Ag-NPs height is only close to ~20 nm thick which is the thickness of the PEDOT:PSS layer. This implies that Ag-NPs of less than 20 nm thick have a limited contribution to the optical absorption increase because their enhanced electric fields are only embedded within the PEDOT:PSS layer.

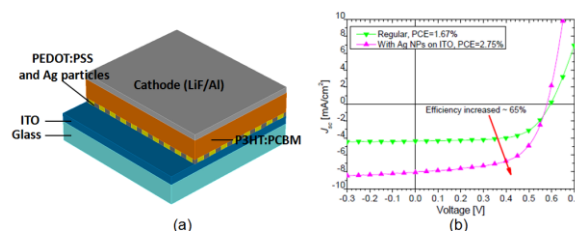


Fig. 1. Device structure (a), and J_{sc} -V characteristics of organic solar cells with and without Ag-NPs (b). The short-circuit current density with Ag-NPs of 5 nm thick was obviously increased due to the enhancement of the photogeneration of excitons near the plasmonic resonance of the Ag-NPs. Parameters such as J_{sc} [mA/cm^2], V_{oc} [V], FF [%], and η [%] are 4.7 mA/cm^2 , 0.59 V, 63.5 %, and 1.67 % for a regular cell, and 8.1 mA/cm^2 , 0.58 V, 58.7%, and 2.75 % for a plasmonic solar cell, respectively.

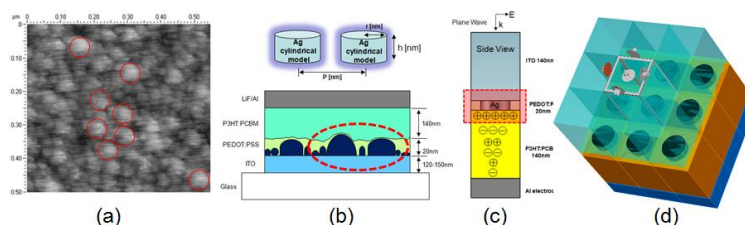


Fig. 2. Schematic diagram of the proposed model. (a) Atomic force microscope of Ag-NPs obtained by depositing 5 nm thick of Ag on ITO substrate showing random array of Ag-NPs or clusters, (b) Our approach to model Ag-NPs as a cylindrical shape, (c) An interested area to calculate the electric field E over a volume of a 10 nm width around Ag-NPs, and (d) 2-D device model showing periodically distributed Ag-NPs.

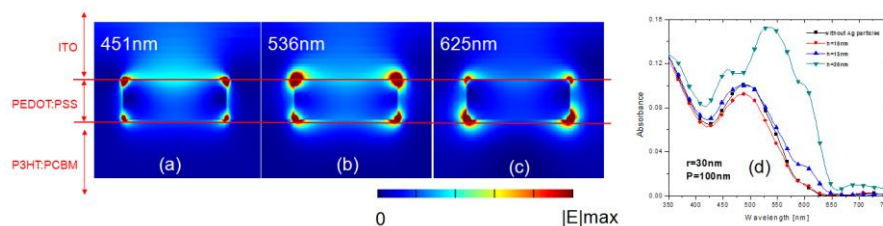


Fig. 3. Simulated electric field intensity enhancement patterns of the Ag-NPs embedded in the PEDOT:PSS/P3HT:PCBM layers at three optical wavelengths. (a)-(c) the optical fields calculated using the finite-difference time-domain (FDTD) method, (d) normalized absorption spectra of the P3HT:PCBM layer with and without Ag-NPs using $r=30\text{ nm}$, $p=100\text{ nm}$, and $h=0\text{ nm}$, 10 nm, 15 nm, 20 nm.

3. Conclusion

We have demonstrated an increased optical absorption in an organic BHJ solar cell originated from LSPRs due to the generated strong electric field, and proposed a theoretical model using cylindrical Ag-NPs based on FDTD analysis which is useful to understand the plasmonic optical enhancement, eventually leading to more photocurrent generation in an organic solar cell.

4. References

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- [2] B. P. Rand et., al, "Long-range absorption enhancement in organic tandem thin-film solar cells containing silver nanoclusters," Journal of Applied Physics 96, 7519-7526, 2004.

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