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Effective medium analysis of thermally evaporated Ag nanoparticle films for plasmonic enhancement in organic solar cell

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ABSTRACT

Films of silver nanoparticles have optical properties that are useful for applications such as plasmonic light trapping in solar cells. We report on the simple fabrication of Ag nanoparticle films via thermal evaporation, with and without subsequent annealing. These films result in a random array of particles of various shapes and sizes. The modeling of such a vast collection of particles is still beyond reach of the modern computers. We show that it is possible to represent the silver island films by the Bergman effective mediums with the same optical properties. The effective medium method provides us with deep insight about the shape, the size and the distribution of nanoparticles. The far field simulations of solar cells, in which the silver island film is replaced with an effective medium layer, show a reduction in the absorption of active layer. Besides, the near field simulations based on finite-difference time-domain technique demonstrate that the near field effects on active layer absorption are negligible and this method highlights the importance of nanoparticles shapes. The PCPDTBT:PCBM solar cells with embedded silver island films are fabricated, and it is found that their performances show the similar trend. This insight can be used for the optical analysis of thermally evaporated Ag nanoparticle films for the improvement of organic solar cells.

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1. Introduction

Organic photovoltaic (OPV) devices have attracted the interest of researchers due to their potential applications as a low cost, high throughput, and flexible source of clean energy [\[1\]](#page--1-0). For the OPV to become commercially reasonable; however, the power conversion efficiency (PCE) must be enhanced further [\[2\]](#page--1-0). The large band gap of the organic semiconductors is one of the limitations, which leads to lower PCE. Currently, high efficiencies have been reported for polymers:fullerene solar cells based on low band gap polymers, such as PCPDTBT [\[3\]](#page--1-0). These polymers have increased light harvesting properties due to their energetically smaller band gaps. The exciton penetration depth in polymers is very small, which leads to a highly thin active layer. So, the light trapping in this type of solar cells should be considered more essentially [\[4\]](#page--1-0). Diverse light trapping structures, including randomly or periodically textured surfaces, photonic and plasmonic structures (such as metal nanoparticles) have been intensively studied in different kinds of solar cells [\[1,2,4,5\].](#page--1-0) The hybrid nature of surface plasmon (SP) modes, propagating surface plasmon polaritons (SPPs) and localized surface plasmons (LSPs), make plasmonic materials attractive candidates for a variety of energy applications [\[6\].](#page--1-0) Several strategies have been proposed to enhance the efficiency of solar cells by using plasmonic metal nanostructures [\[5,7\].](#page--1-0) The first strategy consists of blending the metal nanoparticles (MNPs) into the active layer, for example, by simply mixing a solution containing the dissolved organic semiconductor materials with a colloidal dispersion of the NPs. Despite its simplicity, the findings from this approach are highly controversial as both the enhancement and the detraction in the performance of organic solar cell (OSC) devices have been reported $[8]$. The second strategy is to fabricate OSCs with nanostructured electrodes by either patterning the (semi) transparent front electrode or by reflecting the rear electrode. Generally, this experimental implementation requires more complicated processes and the plasmonic rear-side features are challenging as the processing of OSCs usually begins with the transparent electrode [\[9\]](#page--1-0). The third strategy is distributing MNPs in the hole/electron collection or exciton blocking layer between the active layer and the electrode, either by thermal evaporation [\[10–14\]](#page--1-0) or solution-processing [\[15–17\].](#page--1-0) Consequently, the last strategy can potentially have the advantage of easy fabrication, combined with controlled distance from the active layer, which allows for taking advantage of both near and far field enhancement. Hence, MNPs can be useful as a light scattering center or for enhancing the local field or both, depending upon their size, shape, location and dielectric surrounding [\[18\].](#page--1-0) In addition to the favorable effects for light absorption, MNPs of improper size or shape can give rise to parasitic absorption losses, which reduce solar cell performance [\[8\].](#page--1-0) So, numerical simulations can be beneficial tools for studying and optimizing the plasmonic effects of MNPs in solar cell design.

Ag and Au are the most widely used materials, since their surface plasmon resonances are located in the visible range and, therefore, they interact with the peak of the solar intensity more strongly. Silver is generally considered to have the most suitable optical properties for plasmonic applications in solar cell enhancement. It has a strong resonance and low absorption in the visible and near infrared part of the spectrum [\[19,20\].](#page--1-0)

Thermal evaporation is one of the simplest and most effective physical methods for synthesizing MNPs [\[18\].](#page--1-0) This fabrication technique results in a random array of particles with a variety of shapes and sizes. The modeling of such a vast collection of particles is still beyond the capabilities of modern computers.

As a method of simulation, the full wave methods, like Finite-difference time-domain (FDTD) which solve the Maxwell's equations rigorously, are more accurate but computationally expensive. Consequently, these techniques are mostly limited to a single NP $[21]$ or periodic array of identical NPs [\[22\].](#page--1-0) As a result, approximate models are required to perform optical simulations of this type of NPs [\[23\]](#page--1-0). In this way, despite substantial research activities, studies are missing which, analyze applicability of thermally evaporated Ag NPs in the PEDOT:PSS buffer layer as effective plasmonic layers for enhancing the light absorption of active layer.

In this paper, we fabricate the thermally evaporated Ag NP films (with and without subsequent annealing) between two PEDOT:PSS layers on glass/ITO electrodes. Scanning electron microscopy (SEM) is used to characterize the geometry and surface coverage of the NP films. Afterwards, we

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