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Numerical Study of Plasmonic Effects of Ag Nanoparticles embedded in the Active Layer on performance polymer organic Solar Cells

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Abstract

In this paper, the light absorption the active layer of polymer polymer solar cells (OPV) by using plasmonic nanocrystals with hexagonal lattice is investigated. To study the relation between the performance of the OPV solar cell and its active layer, a three-dimensional model for its morphology is utilized. Therefore, the three-dimensional (3D) finite-difference time-domain method and Lumirical software were used to measure the field distribution and light absorption in the active layer in terms of wavelength. OPV solar cells with bilayer and bulk heterojunction structured cells were designed using hexagonal lattice crystals with plasmonic nanoparticles, as well as, core-shell geometry to govern a design to optimize light trapping in the active layer. The parameters of shape, material, periodicity, size, the thickness of the active layer as a function of wavelength in OPV solar cells have been investigated. A very thin active layer and an ultra-thin shell were used to achieve the highest increase in optical absorption. The strong alternating electromagnetic field around the core-shell plasmonic nanoparticles resulting from the localized surface plasmon resonance (LSPR) suggested by the Ag plasmonic nanocrystals increased the intrinsic optical absorption in the active layer poly(3-hexylthiophene):phenyl-C61-butyric acid methyl ester (P3HT:PCBM). Based on the photovoltaic results the short circuit current ranged from 19.7 to 26.7 mA/cm^2 .

Keywords: Absorption, Finite Difference Time Method, plasmonic Nanoparticles, Organic Solar Cells

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1. Introduction

In the last decade, organic photovoltaic cells (OPVs) have been attracted great attention, due to their promising potential for the next-generation solar cells because they are lightweight, flexible and low-cost, semi-transparency, solution process ability and large surface area [1]. Therefore, OPV solar cells are capable of alternating with conventional photovoltaic devices, since they reduce the cost of energy consumption. Photovoltaic materials are fabricated in thin-film form to decrease the production cost. Various approaches have been employed to enhance light harvesting in the films. Nevertheless, the absorption of light, especially at a long wavelength, is rather low in the OPV solar cells, since they have the thin active layer thickness and indirect bandgap of polymers. consequently, this prevents the cell absorbing low energy photons in the solar energy spectrum [1-2]. Several light trapping and photon management methods have been suggested to improve the performance of OPV solar cells, to improve the collection efficiency of incident light inside thin-films such as antireflection coating [3-4], photonic crystals [5-6], plasmonic excitation using metallic nanoparticles [7], optimization of the electromagnetic field distribution and periodic metallic grating [1,8-9] which are traditionally based on geometrical optics. The efficiency of these polymer cells is low compared to other cells [1], and this is a significant barrier to widespread commercialization of them.

The efficiency of OPV solar cells has been increased by more than 13–14% [4,10]. In OPVs materials, owing to their short diffusion length in the organic semiconductor materials [11], while fairly low carrier mobility ($\sim 10^4 \text{ cm}^2/\text{Vs}$), as well as the photoactive layer is generally rather thin, less than 100 nm to facilitate the charge carrier diffusion and light extraction [10] is achieved. Even though much photon energy is lost, because of the poor absorption of the incident light [11], numerous researches have been done to further light absorption in the OPVs.

Among these approaches, the ideas of plasmonic metallic nanoparticles and gratings play an important role in absorption enhancement. Different kinds of light scattering methods, from random to periodic plasmonic nanocrystals, at the front and/or backside of the active layer, have utilized which light is diffracted, refracted, or reflected back to increase the total path length of incident light inside the active layer.

However, placing metallic plasmonic nanocrystal on top of the active layer would block a huge amount of total incident solar power. Currently, using multiple plasmonic nanocrystal to enhance absorption, on top or/and at the bottom of the active layer, has attracted much attention because of the broadband absorption enhancement, as well as less sensitivity to the angle of incident light [12-13]. Metallic nanoparticles have been exploited to increase the photocurrent, as well as efficiency by 33% of thin-film silicon solar cells [15]. The advantages of the metallic nanoparticles in OPVs have been investigated since they can be used in the device architecture without any significant effort.

Localized surface plasmons (LSP), which are collective oscillations of free electrons in metallic nanoparticles in response to an incident field [3,5], are a type of plasmon, have extensively attracted researchers' attention for different field-enhanced spectroscopy, Photovoltaic and sensing applications [10,7]. In regulation, the light excitation, a resonance, which is named Plasmonic, happens as soon as the frequency of the incident photons reaches the frequency of collective oscillation of conduction electrons of metallic particles, and can interact strongly with external electromagnetic waves [16]. Currently, surface plasmon has become a significant light trapping technique in solar cells [17]. Owing to the near-field nature of the surface plasmons, they are essentially appropriate for application in thin-film devices. Recently, Photonic crystals have also been applied in OPV devices, the same as inorganic solar cells [18-19]. However, this method will be restricted by the relatively low refractive indices of the organic materials since the proper guided modes in photonic crystal devices can be achieved by high index contrast as well as a reasonably thick layer [16-18]. Hence, plasmonic metallic nanoparticles are more appropriate for application in OPV devices [20]. Metallic nanoparticles could enhance scattering and local field from the excitation of localized surface plasmon resonances to improve the OPV performance. Patterned electrodes could enhance local field as well as optical path length by coupling into the surface plasmons to improve the OPV performance. Recently, many papers on plasmonic nanoparticles have been published with applications in OPV technology. The objective of our paper is to use localized plasmons excitation of metallic nanoparticles to trap or confine light inside the photoactive material layer, or to acquire the resonance of the internal light scattering on these plasmonic metallic nanoparticles. This excitation of localized plasmons depends on several parameters, including size, material, the

surface density of the metallic nanoparticles, as well as wavelength, polarization, and incident angle of light. Finally, light absorption could be enhanced, especially in the desired spectral ranges, where the photovoltaic material absorbs the light weakly. For small periods less than 300nm, the reason for improving of the light is mostly LSP [16,19]. The large grating periods could scatter light into surface plasmons [19, 21-22].

The report on performance enhancement through the combination of gold plasmonic nanoparticles in the Poly(3,4-ethylenedioxythiophene): poly (styrenesulfonate) (PEDOT-PSS) active layer has been presented by Chen et al [23] and a 20% improvement has been observed. Ion, et. al. achieved an enhancement in photocurrent due to LSPR generation by embedding the layer of Ag nanosphere between PEDOT-PSS and the active layer P3HT-PCBM of the OPV solar cell [24]. Kulkarni et al. obtained three times more generation of charge carrier by a thin layer of Ag material is inserted at the bottom of the active layer [25]. Zhu et al. reported on the 1.40 times absorption enhancement by plasmonic nanostructures the hybrid active layer and optimizing the fabricated structure [21]. Bai et al. published the first reports on a combination of 2D nanotubes on OPV solar cells, resulting in effective polarization-independent absorption [26]. Diukman et al. showed an improvement in the external quantum efficiency of OPV solar cells after embedding Au nanoparticles arrays in the active layer [27]. Kekeli et al. reported an enhancement in intrinsic optical absorption in the active layer, with and without the square lattice of core-shell (Ag@Sio2) by 24.7% [22].

The Au nanoparticles, which are on the order of 5–50 nm, act as antennas, accumulating incident light energy in localized surface plasmon modes with up to a 100-fold increase in electric field. The generation of a strong near field distribution around the gold nanoparticles embedded in the active layer was simulated and gained an enhancement on the light absorption [17]. These plasmonic nanostructures immersed in the active layer can improve the plasmon and exciton coupling, as well as the generation of hot excitons This generation can enhance the free charges [28-30].

In this paper, to increase the efficiency of polymer solar cells using surface plasmon, factors such as the size and material of plasmonic nanocrystals and the effect of these factors on parameters such as absorption and intensity distribution of electromagnetic fields in the active layer of polymer solar cells are investigated.

In section 2, the theoretical and modelling method, as well as simulation layout, is studied in detail. In the third section, the optical effects of plasmonic nanoparticles

in OPV solar cells are investigated, including: Various morphology size and material of this plasmonic nanocrystal in the active layer of polymer solar cell with bulk heterojunction. The effects of plasmonic nanocrystals on the efficiency of the OPV solar cell by trapping the incident light into the active layer is investigated. Tuning the morphology of a plasmonic nanostructure to achieve higher efficiency is one of the key issues in our research.

2. Theoretical and Simulation Methods

2.1 metallic nanoparticles

Metallic nanoparticles are investigated as plasmonic structures since the LSPR could be tuned by their physical properties such as size, material and shape. These nanostructures can increase the light absorption by cumulative forward scattering cross-section, as well as near-field light enhancement. When the size of the metallic nanoparticles is equal to or smaller than the incident light wavelength, a strong interaction happens among the electromagnetic field with the free conduction electrons in the metallic nanoparticles [31].

Surface plasmon resonance is the collective oscillations in the electron density at the metal surface due to their interaction with the incident light. The resonance happens when the light coupled to the electrons oscillating at the same wavelength, referred to as LSPR in nanostructures and results in a strong enhancement of the localized electromagnetic field. Surface Plasmons, which are coupled with photons, can excite a collective of conduction electrons to propagate along with an interface between a metallic nanostructure and a dielectric with $\epsilon_d > 0$ [31]. The LSP at the vicinity of the interface can be propagated along the metal surface until the energy dissipates. Metallic nanoparticles with a small amount of inter-band absorption, the dielectric function is defined by the Drude and Lorentz model, which elucidates the response of damped and free electrons to an applied electromagnetic field [32]:

$$\epsilon_m(\omega) = \epsilon_r(\omega) + i\epsilon_i(\omega) \quad (2.1)$$

$$\epsilon_m(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)} + \omega_{IB}(\omega) \quad (2.2)$$

The coupling strength between photons and the LSPR is determined by the absorption and the scattering cross-sections of the nanoparticles [33]. In equation 2.2, the Drude model for metal is used to describe the inter-band transition [34]. ω_p is called the plasma frequency and is defined by $\omega_p = \left(\frac{N_e e^2}{m_e \epsilon_0} \right)^{\frac{1}{2}}$, which N_e is the density of free electrons, e is the charge, m_e is the mass of electrons, ϵ_0 is the dielectric constant in free space, γ is the attenuation constant. The second term in Equation 2.2, the Lorentz, describes the inter-band transition for particles, such as holes in the occupied or unoccupied states [31]. The Electronic inter-band transitions significantly influence the surface plasmon resonance in metallic nanoparticles. As soon as the nanoparticle size is much smaller than the incident wavelength, the scattering (C_{scat}) and the absorption (C_{abs}) cross-sections of spherical nanoparticles can be defined as follows:

$$C_{scat} = \frac{1}{6\pi} \left(\frac{2\pi}{\lambda} \right)^4 |\alpha|^2 \quad (2.3)$$

$$C_{abs} = \frac{2\pi}{\lambda} \text{Im}[\alpha] \quad (2.4)$$

$$\alpha = 4\pi a^3 \left(\frac{\epsilon_m - \epsilon_d}{\epsilon_m + 2\epsilon_d} \right) \quad (2.5)$$

Where α is the polarizability of the spherical nanoparticle with radius a , ϵ_m is the dielectric constant of the metal, ϵ_d is the dielectric constant of the environment. If resonance occurs in the system when the following condition is met and the denominator of Equation 2.5 tends to zero [34,35]. If $\epsilon_m = -2\epsilon_d$, the polarization of the particle turns out to be considerable, and the frequency is the same as the SPR ω_{sp} permitting light to interact over a bigger region than the cross-section of the nanoparticle. The scattering efficiency can be calculated using the following formula:

$$Q_{scat} = \frac{C_{scat}}{(C_{scat} + C_{abs})} \quad (2.6)$$

Silver nanoparticles in the air have a scattering cross-section approximately ten times larger than larger particles, allowing them to fully absorb and scatter incident light with just ten percent metallic nanoparticles covering the substrate [34]. Therefore, the bigger the scattering cross-section, the more light trapping is happened by a scattering effect, and more important than the light absorption. The

particles bigger than 100 nm, this effect can be achieved and is suitable for the solar cell device. In addition, the shape, material of the particles, and surrounding medium contributed to enhancing the scattering effect [10,36-38]. Metal nanoparticles directly increase the absorption in the solar cells, which occurs through coupling to near fields [34]. In addition, the absorption in the near field of metal nanoparticles is about hundreds or thousands of times higher than in the surrounding field. The near field strength around nanoparticles depends on the following factors [39]: the stored energy in plasmonic modes, the sharpness and edge of the nanostructure, hence the sharper the edges in the nanostructure, the higher the near field strength around it. The stored energy also depends approximately on the cross-sectional area of the absorption on quasi-static particles (where the size of the particle is much smaller than the incident photon wavelength) [40].

Generally, metallic nanoparticles are made of silver, aluminum, gold or copper due to their strong light. SPR of aluminum and silver occurs in the ultraviolet region, while SPR of gold and copper happens in the visible region [35]. Mostly, silver nanoparticles for their low cost as well as low absorption are employed in OPV, although gold nanoparticles have recently been largely used due to not having oxidation effects.

Although the use of nanoparticles in solar cells increases the absorption of photons in the cell, mostly, a semiconductor is coated on the nanoparticles to protect them from corrosion and recombination. Semiconductors such as TiO_2 , SiO_2 and Al_2O_3 coated on gold and silver nanoparticles as a protective layer are employed in the solar cells [41]. Altering the thickness of the coating layer and the dielectric of the surrounding environment (ϵ_d) and the dielectric constant of the coating layer (ϵ_c) are influenced by the resonance, Therefore the thickness of the coating layer increases, the resonance shifts toward the higher wavelengths. Consequently, the longer the wavelength, the greater the number of photons and the higher the intensity can be achieved. The wavelength intensity and position of the SPR depend on the dielectric function of the metal and is expressed by Equation 2.2 [31,34].

2.3 The Finite Difference Time Domain (FDTD) Method

In this method, the understudied structure and interacting fields are defined by discretizing the simulation space and allocation of optical properties to cells of the

mesh. The technique was introduced in 1966 by YEE [42] but did not receive much attention until the late 1980s owing to lack of access to computers with adequate speed and memory.

Fig. 1 Gridding in 3-dimensional FDTD space and position of components of electric and magnetic fields onto each cell

With advances in the production of personal computers, this technique came to prominence for studying propagation and interaction of electromagnetic waves and matter in many branches of science, including: physics, electronics, communications, photonics, etc. [43].

In the standard FDTD method, simulation space is divided into identical cubic cells as shown in fig. 1. Positions of components of electric and magnetic fields on each cell are alternately determined in a way that each component of the electric field is enclosed by components of the magnetic field and vice versa. By discretizing Maxwell's equations through applying finite-difference on spatial and time components of the field, six updating equations are achieved for six components of electric and magnetic fields.

The structure is discretized with a non-uniform grid mesh, which is subdivided into rectangular unit cells. The H- and E-field are shown in time steps, where during each time step they are iteratively updated. To avoid the reflections at the domain boundary, perfectly matched layers (PML) are applied. A three-dimensional non-uniform lattice is introduced as follows. The vertices of the lattice are defined by the one-dimensional coordinates:

$$\{x_i, i = 1, N_x\}; \quad \{y_j, j = 1, N_y\}; \quad \{z_k, k = 1, N_z\} \quad (2.7)$$

The cell and edge centers in the non-uniform space are introduced as:

$$x_{i+1/2} = x_i + \Delta x_i / 2; \quad y_{j+1/2} = y_j + \Delta y_j / 2; \quad z_{k+1/2} = z_k + \Delta z_k / 2 \quad (2.8)$$

The E- and H-field in the non-uniform grid are denoted as follow:

$$\begin{aligned} E_x \Big|_{i+1/2,j,k}^n &\equiv E_x(x_{i+1/2}, y_j, z_k, n\Delta t) \\ H_x \Big|_{i,j+1/2,k+1/2}^{n+1/2} &\equiv H_x[x_i, y_{j+1/2}, z_{k+1/2}, (n+1/2)\Delta t] \end{aligned} \quad (2.9)$$

This algorithm is based on a discretization of Maxwell's equations in their integral form [16]. The surface integrals are performed over a lattice cell face, and contour integral is performed over the edges bounding face. The equation over cell faces using the discrete field approximations in Equation (2.9) and evaluating the time derivatives using central difference approximations leads to:

$$\begin{aligned} E_x \Big|_{i+1/2,j+1,k}^n \Delta x_i - E_x \Big|_{i+1/2,j,k}^n \Delta x_i - E_y \Big|_{i+1,j+1/2,k}^n \Delta y_j + E_y \Big|_{i,j+1/2,k}^n \Delta y_j = \\ - \left[\mu_{i+1/2,j+1/2,k} \left(\frac{H_z \Big|_{i+1/2,j+1/2,k}^{n+1/2} - H_z \Big|_{i+1/2,j+1/2,k}^{n-1/2}}{\Delta t} \right) + M \Big|_{i+1/2,j+1/2,k}^{n+1/2} \right] \Delta x_i \Delta y_j \end{aligned} \quad (2.10)$$

$$\begin{aligned} H_x \Big|_{i,j+1/2,k+1/2}^{n+1/2} h_{x_i} - H_x \Big|_{i,j-1/2,k+1/2}^{n+1/2} h_{x_i} - H_y \Big|_{i+1/2,j,k+1/2}^{n+1/2} h_{y_j} + H_y \Big|_{i-1/2,j,k+1/2}^{n+1/2} h_{y_j} = \\ - \left[\epsilon_{i,j,k+1/2} \left(\frac{E_z \Big|_{i,j,k+1/2}^{n+1} - E_z \Big|_{i,j,k+1/2}^n}{\Delta t} \right) + \frac{\sigma_{i,j,k+1/2}}{2} \left(\frac{E_z \Big|_{i,j,k+1/2}^{n+1} + E_z \Big|_{i,j,k+1/2}^n}{\Delta t} \right) + J \Big|_{i,j,k+1/2}^{n+1/2} \right] h_{x_i} h_{y_j} \end{aligned} \quad (2.11)$$

Where $h_i^x = (\Delta x_i + \Delta x_{i-1})/2$; $i = 2, N_x$ and the other component is introduced in the same manner. $\epsilon_{i,j,k+1/2}$, $\sigma_{i,j,k+1/2}$ and $\mu_{i+1/2,j+1/2,k}$ are the averaged permittivity, conductivity and permeability about grid edges, respectively. Similar updates for other components are easily derived.

Particularly for three dimensions simulation, this process is very time-consuming and requires a lot of computer memory resources. To acquire good stability between accuracy and computational resources, 10 grid points per lattice constant "a" is utilized. Several detectors are used to record the electric and magnetic fields of light. A commercial 3D-FDTD code is used, (Lumerical) to enable us the free positioning, moving, and tilting of the structure. The power flow is calculated as follows:

$$S = \frac{\int (\vec{E}_0 \times \vec{E}) d\vec{A}}{\int (\vec{E} \times \vec{E}) d\vec{A}} \quad (2.12)$$

2.3 OPV Solar Cells

Organic Solar Cells, which are called Organic Photovoltaics (OPV), have been considerably used by industry and researchers in the recent past [44-47]. The five critical procedures for an effective OPV are summarized as 1. Light absorption goes together with exciton's creation, 2. Diffusion of the excitons through active layer interface, 3. the dissociation and separation of charge, 4. Transporting the separated charges, 5. Charge gathering (fig. 2) [48].

Fig. 2 Schematic of OSC principle operation

Carbon-based organic compounds, or polymers are commonly used as active semiconducting materials in organic or polymer solar cells, which can convert solar energy into electric energy. Three types of OPV are categorized as single-layered, bilayer, and bulk heterojunction structured cells. The first group of OPVs is mainly made of single organic layers inserted between two metal electrodes [49]. Since the tremendously low charge separation is caused by the presence of tightly bound excitons in organic semiconductors, these layers, as p-type or n-type sandwiches between electrodes are non-capable of appropriately creating charges in the single-layer structure [50]. Kippelen B et al. reported single-layer OPVs with efficiencies as high as 5.9% recently [51].

In bilayer/multilayer OPVs, the active layers containing donor and, acceptor organic semiconductors absorb light and as a result, generate photocurrents. The donor material is capable of donating electrons, resultant holes, while the acceptor materials can accept electrons. Photons from light are collected by these active layers to form excitons, which produce a concentration gradient, to diffuse them towards

the donor or acceptor interface and separate them into free holes and electrons. Therefore, free electrons and holes transfer to the electrodes, resulting in photovoltaic. In a bilayer heterojunction device, p and n-type materials are consecutively placed with each other [50].

The third one, bulk heterojunction is arranged by bulk volume mixing of donor and acceptor components, which outcomes in very slight exciton diffusion length at their interface [49]. Excitons are formed as soon as photons are absorbed by organic materials. Finally, separation of excitons bounces charge gathering at the heterojunction interface at the electrodes, resulting in photovoltaic [50].

Although the inorganic semiconductor has a suitable bandgap, the main problem with them is, they possess less light absorptivity than organic materials [44]. Therefore, inorganic semiconductors require a bigger absorbing layer, producing thicker devices. Moreover, one of the vital features of inorganic semiconductors is purity in attaining higher performance, which increases the cost of production. The inorganic semiconductors, alternatively, have a lower energy bandgap for creation of excitons to produce charge carriers. As a result, for fabricating OPVs, we should attempt better electron and hole mobility, which will consequence in higher performance.

2.4 MODEL CONFIGURATION

Fig. 3 depicts the schematic structure of an OPV solar cell, where a hexagonal periodic array of nanoparticles is embedded inside the P3HT: PCBM active layer on the top of aluminum. The PML boundary conditions on the bottom of the aluminum layer were used to avoid reflections in the stack direction. To create multiple scattering and cross-linking between adjacent nanoparticles, the boundary conditions along the X and Y directions were considered periodically. The simulation mesh size was fixed at 0.5 nm in the region encircling the nanoparticles. The plane wave was illuminated at the normal incidence along the z-direction to propagate through the structure, with a wavelength range between 300 and 900 nm. The OPV solar cell is designed of three thin layers, which includes an aluminum substrate as a cathode with a thickness of 100 nm, the active layer of poly trihexyl thiophene (P3HT: PCBM) with a thickness of 40 nm, a highly conductive polymer

layer, and the polyethylene dioxide thiophene: polysulfonate (PEDOT: PSS) as the anode with a thickness of 30 nm and also plasmonic metal nanospheres were used as a hexagonal lattice. The refractive index (n for the real part and refractive index k for the imaginary part) PEDOT: PCBM and P3HT: PCBM is taken from Ami abass [52]. To enhance the performance of OPV solar cells by improving light absorption, plasmonic nanocrystals were employed as a hexagonal lattice inside only the active P3HT: PCBM layer (as shown in Fig. 3). Intrinsic adsorption inside the active layer is calculated without silver material absorption on plasmonic nanocrystals. Furthermore, the increase in optical absorption in multilayer cells can be evaluated to high efficiencies.

For this calculation, the dissipated power $L(\lambda)$ into the volume (x, y, z) of material from the Poynting vector $\Pi(x, y, z, \lambda)$ is expressed as following [16]:

$$L(\lambda) = \int^x \int^y \int^z -\text{div} \{(\Pi(x, y, z, \lambda))\} dx dy dz \quad (2.13)$$

The intrinsic absorption $A(\lambda)$ in each layer is governed by the ratio of the $L(\lambda)$ in each volume to the total power of the incident light source $P_{\text{Source}(\lambda)}$ as following (2.14) [53]:

$$A(\lambda) = \frac{L(\lambda)}{\text{source}(\lambda)P} \quad (2.14)$$

In the wavelength range of 300 to 900 nm, the optical absorption enhancement A_E is calculated as follows (2.15) [54]:

$$A_E = \frac{\int_{\lambda_2}^{\lambda_1} \left(\left(\frac{\lambda}{hc} \right) A(\lambda) I(\lambda) d\lambda \right)}{\int_{\lambda_2}^{\lambda_1} \left(\left(\frac{\lambda}{hc} \right) A_{\text{without NSs}}(\lambda) I(\lambda) d\lambda \right)} \quad (2.15)$$

Where, h is Planck's constant and c is the speed of light in vacuum, while $I(\lambda)$ denotes the AM_{1.5}G solar spectral irradiance. $A(\lambda)$ and $A_{\text{without NSs}}(\lambda)$ are the intrinsic optical absorption (inside the active layer) with and without nanospheres, respectively. The dissipated power (D_p) via the active layer of the plasmonic nanocrystal of intrinsic absorption is defined by the AM_{1.5}G illumination of light in the wavelength range of 300 to 900 nm [55].

$$D_p = \int_{\lambda_2}^{\lambda_1} A(\lambda) I d\lambda \quad (2.16)$$

The square of the electric field integration over the volume is employed for the calculation of the absorption of the total energy of light by the substrate.

$$Q_{\text{with(without)}}(\omega) = \frac{\omega}{4\pi} \int_V n_3 \varepsilon''_{\text{with(without)}}(\omega) E^2 \quad (2.17)$$

This denotes the imaginary part of the dielectric function of the substrate with and without metallic nanoparticles. The ratio of light absorbed with and without metallic nanoparticles is defined as the light absorption (efficiency).

$$A(\omega) = \frac{Q_{\text{with}}(\omega)}{Q_0(\omega)} \quad (2.18)$$

Finally, there is the absorption enhancement. For the measurement of the induced short circuit current I_{SC} in the cell (the presence of metallic nanoparticles), an integration over the solar spectrum is used:

$$I_{\text{SC}} = \frac{\int Q_{\text{with}}(\omega)F(\omega)d\omega}{\int Q_0(\omega)F(\omega)d\omega'} \quad (2.19)$$

where $F(\omega)$ represents the AM1.5 G solar light.[56]

Fig. 3 a shows the structure of the reference cell. the structure of a polymer solar cell with plasmonic nanocrystal in a hexagonal lattice in three dimensions. b Schematic of the proposed multilayer structure and simulation layout. The boundary condition is shown.

3. RESULTS AND DISCUSSIONS

The metallic nanoparticles embedded on the OPV solar cell in three dimensions are simulated using Lurmical FDTD and their plasmonic effect analyzed as the model configuration is shown in Fig. 3 a and b. The period, size, and material of Ag nanoparticles are varied to study how these nanoparticles could enhance the light absorption of the OPV solar cells. The results of the simulation are illustrated in Fig. 4,5,6,7,8,9,10. The photon absorption spectrum of OPV solar cells is plotted with and without Ag nanoparticles located inside the P3HT: PCBM in terms of wavelength at normal incidence. The simulation makes it possible to optimize the amount of light scattered into the P3HT: PCBM for several materials, periods and sizes of the metallic nanoparticles. Several parameters such as: material, alternating period and size of Ag nanoparticles, the thickness of polymer active layer, as well as dielectric shell with different thicknesses around Ag nanoparticles were investigated in detail. The wavelength range from 300 nm to 900 nm is taken into account here.

3.1. Ag nanoparticles embedded inside the P3HT: PCBM layer

The comparison of light absorption of OPV solar cell with and without Ag nanoparticles revealed that the Ag nanoparticles in a hexagonal array embedded inside the P3HT: PCBM layer increased the plasmonic effect on the light absorption of OPV solar cell. Recent papers have shown that the LSP mode, which traps induces light, enhances the light absorption with plasmonic metallic nanoparticles, and their electric field inside the metallic nanoparticles is proportional to that outside [17,57]. Hence, the light absorbed inside the Ag nanoparticles, traps most of the incident light and is absorbed by the active layer of the OPV solar cell. The peak of increase in absorption due to plasmonic nanosphere crystals is observed at approximately 680 nm. Moreover, an additional spectral peak is observed at 620 nm. These peaks result from the LSPR between neighbouring Ag nanoparticles hexagonal array, as is shown in Fig. 3. Fig. 7 demonstrates the thickness dependence of the absorbance spectra. The increase in light absorption is due to the increase of the near field in the active P3HT: PCBM layer. The magnetic field distribution is shown in Fig. 4, The enhanced field between the plasmonic nanospheres is polarized in the direction of light.

Fig. 4 The absorption spectrum of OPV solar cell with and without Ag nanoparticles located inside the P3HT: PCBM.

Fig. 5 The field profile of exciting mode defined for OPV solar cell with Ag nanoparticles located inside the P3HT: PCBM.

3.2 Effect of Period on Absorption Enhancement

The OPV solar cells were simulated with periodic arrays of Ag nanoparticles (with a radius of 15 nm and 25-55 nm period) embedded inside the P3HT: PCBM layer active. The effect of plasmonic enhancement by altering the period of absorption is displayed in Fig. 6. By tuning the period and size of the Ag plasmonic nanocrystals, the SPR peak can be designed to optimize the absorption of the whole incident light in the active polymer layers. Fig. 6 shows the absorption on the polymer active layer as a function of the Ag plasmonic nanocrystals period. This parameter displays the most effects on near field enhancement in Ag plasmonic nanocrystals. When the period of the nanoparticles array is much larger than the size of the nanoparticles, the absorption factor decreases, since the field scattering of the adjacent nanoparticles in the further distance is weaker. As the period of the nanoparticle array reduced, the absorption factor enhanced, as long as it reached a maximum value in a suitable period. This maximum value occurs where the field scattering is very large, where the nanoparticles are coupled to the electromagnetic field. [22,58]. As it is clear in fig 6, the optimal period of Ag plasmonic nanocrystals was observed

around 25 to 30 nm.

Fig. 6 Absorption of the Ag plasmonic nanocrystals with the diameter of 15 nm embedded inside the 40 nm thick P3HT: PCBM active layer in terms of different alternating periods.

3.3 Effect of Plasmonic Nanocrystals Size

The radius of the plasmonic nanocrystal is another significant parameter. As the radius of the Ag plasmonic nanocrystal increased, the absorption peak enhanced and shifted to higher wavelengths, as is shown in Fig. 7. It can be concluded that with growing the size of the plasmonic nanocrystal, the absorption, as well as the scattering cross-section increased.

Fig. 7 Absorption of the Ag plasmonic nanocrystals with the diameters of 5, 10, 15, 20 nm and a period of 25 nm embedded inside the 40 nm thick P3HT: PCBM active layer in terms of wavelength.

3.4 Effect Material Plasmonic Nanocrystals

The absorption factor in terms of wavelength for different plasmonic nanocrystals is shown in Fig. 8. Hexagonal array of plasmonic nanocrystals with different materials such as silver, gold, aluminum, and copper embedded inside the P3HT: PCBM active layer are investigated. The results revealed that silver is the best material with higher absorption [59]. An interface Schottky barrier is formed between Ag, Au and others, since the nanoparticles are adjacent to each other. Its depth depends on the metal sizes, work functions, and accordingly, the induced electron transfer, as well as the efficiency would be higher. The separation of excited charges in the presence of an electric field improved the device's efficiency for the solar energy application. The work function 5.1 4.26, 4.67, and 4.18 e v for Au, Ag, Cu, and Al, respectively. As a result, Au with higher work function is more active, while their morphology, the incident light intensity, as well as excitation wavelength influence electron transfer. As long as the excitation is shifted to a higher wavelength, the steady-state polarization is increased, while the Fermi levels are shifted to reach the conduction

band of their embedded medium to enhance charge transport. The size of the metallic nanoparticles is shifted the Fermi level to upward or downward. Since nanoparticles are well attached to the surface of the embedded medium in comparison to the large particles, thus, the Fermi level is shifted from more negative level, which could be tuned to a appropriate location by choosing and controlling the actual material, shape, as well as, size of the metallic nanoparticles.

Fig. 8 Absorption of the Ag plasmonic nanocrystals with the diameter of 15 nm and period 25 nm embedded inside the 40 nm thick P3HT: PCBM active layer in terms of wavelength.

3.5 Effect of the Polymer active layer Thickness on Absorption Enhancement

The absorption plasmonic nanocrystals in the P3HT: PCBM active layer is simulated as a function of the thickness of the active layer, as shown in Fig. 9. The P3HT: PCBM layer usually makes better hole transport from the active layer to the anode, This active layer is presented in the OPV solar cell with a thickness of 40 nm. The thickness variation of the P3HT: PCBM active layer from 20 to 70 nm is chosen, which has not observed substantial improvement from 40 to 70 nm on the absorption

in the P3HT: PCBM active layer, as shown in Fig. 9. However, as the thickness of the P3HT: PCBM active layer increases from 20 nm to 70 nm, the amount of absorption increases. By the growing thickness of the active layer, the multiple peaks correspond to the LSPR inside or between neighbouring holes. In addition, the resonances get weaker as thickness grows due to less light-matter interaction. Therefore, we expect that the sensitivity to the thickness variation in the optimum active layer is small.

Fig. 9 shows the light absorption of an OPV solar cell in terms of the thickness of the polymer active layer.

3.6 Effect of The Hexagonal plasmonic nanocrystals Shell Thickness on Absorption Enhancement

Finally, the increase of light absorption is investigated by using plasmonic nanocrystals of silver nanospheres with dielectric shells. In some electron-hole recombination materials from plasmonic nanocrystals in application systems, they may significantly reduce conversion efficiency by LSPR, another reason for the use of nanoshells in applications to prevent plasmonic nanoparticles corrosion. To solve this problem, nanospheres are separated from the active polymer layer by dielectric shells.

Dielectric shells with different refractive indices and thicknesses also change the location of the SPR peak [60]. Figure 8 shows the absorption factor in the P3HT: PCBM active layer as a function of shell thickness using two dielectric shells made of SiO_2 , and Al_2O_3 . The absorption factor decreases with increasing thickness for both shells. This decrease is more severe for SiO_2 than for Al_2O_3 . This is because the change in shorter wavelengths for silicon dioxide is larger than for Al_2O_3 , and this is because SiO_2 has a smaller refractive index.

Fig.10 Absorption of the Ag plasmonic nanocrystals with the diameter of 15 nm and period 35 nm embedded inside the 40 nm thick P3HT: PCBM active layer in terms of dielectric shell thickness of SiO_2 , and Al_2O_3 .

As a result, the surface plasmon resonance improves the enhancement of the scattering and absorption cross-sections of the metallic nanoparticles. Meanwhile, scattering and absorption procedures are happened, through radiative and nonradiative plasmon decay processes, respectively, their decays rate ratio depends on the nanoparticles morphology nanoparticles. The radiative plasmon decay originates from the scattering, and it is more usual in Ag nanoparticles with larger sizes. The nonradiative plasmon decay originates from the absorption, which leads to the robust absorption of light and happens via intra-band excitations within the conduction band or inter-band excitations below the conduction band. It is more

common in smaller sizes of Ag nanoparticles. The robust absorption of light leads to more electron-hole pairs production, consequently, enhances the light absorption, as well as efficiency of the OPV solar cell.

3.7. Photovoltaic performance

As discussed later, absorption enhancement is mostly attained in the short wavelength range using hexagonal Ag plasmonic nanocrystals embedded inside the P3HT: PCBM active layer in fig 2. Although Ag plasmonic nanocrystals influence the short wavelength region, the main enhancement occurs at long wavelengths. OPV solar cell fabrication using Ag plasmonic nanocrystals as an absorber in the active layer is analyzed by using the advantage of the density of state of Ag plasmonic nanocrystals by arranging their bandgap in the non-absorbing region at the weakly absorbing region. Table 1 summarized the characteristics of the I-V curve of the OPV solar cell structure with and without Ag plasmonic nanocrystals. It shows a clear improvement in J_{SC} of the OPV solar cells in comparison to the cell without Ag plasmonic nanocrystals as a reference cell. Moreover, the characteristics of the I-V curve of all the proposed OPV solar Cells are calculated and the results are presented in Table 1. The results revealed that all physical parameters influence on absorption enhancement, J_{sc} and consequently, the efficiency of OPV solar cells.

Table 1: Summary of the OPV solar cell's performance.

Proposed OPV Structure With P3HT: PCBM active layer	J_{SC} (mA/cm ²)	Absorption Enhancement (%)
Without Ag plasmonic nanocrystals (Reference)	19.7	---
With Ag plasmonic nanocrystals	24.3	26.6
Core Ag, dielectric shell SiO ₂	25.12	26.1
Core Ag, dielectric shell Al ₂ O ₃	25.01	26.0
thickness of the polymer active layer 20	11.6	-34.2
thickness of the polymer active layer 50	16.9	-14.6
thickness of the polymer active layer 70	24.0	26.3
thickness of the polymer active layer 80	26.7	32.7
materials: silver nanoparticles	24.3	26.6

materials: gold nanoparticles	24.6	26.9
materials: aluminum nanoparticles	24.7	27
materials: copper nanoparticles	24.2	26.4
radius of Ag nanoparticles 2.5 nm	19.8	3
radius of Ag nanoparticles 5 nm	21.3	15.4
radius of Ag nanoparticles 7.5 nm	23.1	19.5
radius of Ag nanoparticles 10 nm	24.4	26.8
Period of Ag plasmonic nanocrystals 25 nm	23.5	24.8
Period of Ag plasmonic nanocrystals 30 nm	26	31.4
Period of Ag plasmonic nanocrystals 35 nm	23.7	21.6
Period of Ag plasmonic nanocrystals 45 nm	20.5	12.1

Conclusion

Light absorption enhancement by an Ag plasmonic nanocrystals hexagonal array embedded inside the P3HT: PCBM active layer at the bottom of the OPV solar cell was analyzed. FDTD simulations were performed to further investigate the influence of different geometry parameters on the absorption enhancement. Simulation results revealed that Ag plasmonic nanocrystals can significantly improve total absorption by exciting numerous optical resonances. The outcome of each active layer and nanoparticle morphology design on the absorption enhancement was debated. Light scattering by Ag plasmonic nanocrystals enhances light absorption in the long wavelength range, and also generates a strong electromagnetic field.

As proved in the simulation, plasmonic nanostructures with various morphology parameters such as size, materials, display different behavior on absorption enhancement. For instance, a different range of Ag nanoparticles embedded in the P3HT: PCBM active layer, using Lumerical FDTD, makes it possible to estimate the amount of light scattered into the P3HT: PCBM active layer for various materials and sizes of the Ag nanoparticles. It was seen that the scattered light scattered inside the active layer was influenced by the size, the material, and embedded environment of the Ag nanoparticle. Finally, the resonant plasmon excitation in an OPV solar cell is to exploit the strong local field enhancement around the Ag nanoparticles, which improves the light absorption in the P3HT: PCBM active layer. In conclusion, we have revealed that the I_{SC} , consequently, efficiency, was enhanced due to light scattering, strong absorption and the resonant plasmon excitation of Ag plasmonic

nanocrystals. The clear enhancement in the I-V curve is attained with the Ag plasmonic nanocrystals embedded in the active layer of the OPV solar cells.

Conflict of Interest

The authors declare that they have no conflict of interest.

Ethical approval

This paper does not contain any studies with human participants or animals performed by any of the authors.

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Authors' contributions

A. Mohammadi designed and directed the project, and with L. Shabani, contributed to the design and implementation of the research, A. Mohammadi, L. Shabani, T. Jalali contributed to the analysis of the results and to the writing of the manuscript.

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Data and code availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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