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اثر نانومیله های پلاسمونیکی فلزات نجیب طلا و نقره بر جذب موثر در سلول خورشیدی لایه نازک آلی P3HT:PCBM

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چکیده – در این مقاله با استفاده از روش تفاضل محدود زمانی ، سلول خورشیدی آلی ، با لایه فعال *P3HT:PCBM* و وارد کردن نانو میله های فلزی طلا و نقره در لایه فعال، شبیه سازی شده است.همچنین در این مقاله با بررسی نمودار های جذب و چگالی جریان و افزایش میدان در اطراف نانو ذرات وارد شده، مکانیزم اثر نانو ذرات بر افزایش پارامتر های اشاره شده، مورد بررسی قرار گرفته است.نشان داده می شود، در فرکانس رزونانس پلاسمون برای نانو ذرات فلز وارد شده به علت افزایش میدان نزدیک و همچنین پراکندگی ، مقدار جذب و چگالی جریان به طور چشم گیری افزایش می یابد. همچنین با بررسی دوره تناوب های مختلف، یک مقدار اپتیمم برای جذب و چگالی جریان بدست آمده است.

کلید واژه- افزایش جذب در سلول خورشیدی، پلاسمون سطحی، پراکندگی نور، سلول خورشیدی آلی.

Plasmonic noble metal Gold and silver Nano rods effect on efficient absorption in thin film organic solar cell P3HT: PCBM

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Abstract- In this paper an organic solar cell by P3HT: PCBM polymer active layer with gold and silver Nano rods within active region, with Finite Different Time Domain method has simulated. Also the mechanism of Nano rods effect on enhancement of absorption, current density and near field parameters has studied. We will demonstrate that due to the increasing in near field and scattering surround the Nano rods, absorption and current density will increase alternatively. Also we investigate an optimum absorption and current density for various periods of Nano rods in active region.

Keywords: absorption in solar cell, organic solar cell, scattering, surface Plasmon.

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Plasmonic noble metal Gold and silver Nano rods effect on efficient absorption in organic solar cell P3HT: PCBM

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1 . Introduction

Increasing efficient absorption, in organic solar cells is a major issue, because of their advantages such as low cost and easy fabrication[1]. There is some method to reach this approach, such as using metal nanoparticles as localized surface Plasmon (LSP), in various layers of solar cell, to improve absorption in active layer [2].

The metal nanoparticles, scatter and couple incident light and confine the light surrounding their surfaces [3, 4]. When particles size is smaller than wavelength, metal will show some properties in plasma resonance that behaves like plasma of gases, led to enhancement the field near metal nanoparticles in active region. The first effect of decreasing metal particle's size to smaller scale of incident light is that, the atoms on the surface have more impression on properties of metal than the atoms in volume. Because of free electron oscillation on metal nanoparticles, they are highly reflective at plasma resonance frequency.

Metal Nano rods when illuminated, support LSP modes [5]. These plasmonic excitations have tow pathways to decay: 1) nearfield effect that led to increase in electric field amplitude and intensity near nanoparticles and. 2) far field effect that will increasing in field because of strong scattering by metal nanoparticles [6]. Thus interaction between incident light and LSP, change the optical properties of active region. The physical discussions, of scattering by metal nanoparticles come from electric dipole concept [7].

For gold and silver, by increasing wavelength, Re(ε_p) decreases and Im (ε_p) increases at resonance frequency. Then the absorption spectra peaks will red shift by increasing ε_m (dielectric function in medium) [8].

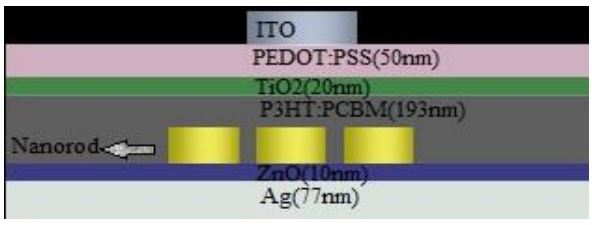
The wavelength of surface Plasmon polariton(SPP) depends on length of nanoparticles(L) and mode index(m) as indicated in equation (1) [9]:

$$\lambda_{spp} = \frac{2L}{m} \qquad (1)$$

2. Simulation and theory

In this simulation we used FDTD[1] method, to simulate thin film organic solar cell. The active region is poly (3-hexylthiophene) and phenyl-C61-butyric acid methyl ester (P3HT: PCBM) by thicknesses of 193nm that is interested from 300nm to 800 nm of solar spectrum. We need to generate electron-hole pairs in this layer and then separate them in electrodes to produce current in solar cell. We used transparent Indium Tin Oxide (ITO) Nano wire as top electrode to collection holes. Also for better hole transfer to ITO we used 50 nm thicknesses of poly (3, 4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT: PSS) polymer and 20nm thickness of Titanium Oxide (TiO2), because of their band position for hole transfer.

Also we used 77nm thicknesses silver (Ag) as back electrode to collect electrons generated in active layer. And for good electron transfer ability of Zinc Oxide (Zn O) we used 10 nm thicknesses of this layer. Also in active layer, we used silver and gold Nano rods in 3*3 arrays with three various periods, 250 and 300 and 350 nm(each period is distance of tow Nano rods centre) and Each Nano rod has 150 nm height and its radius is 120 nm, as showed in figure (1), to reach high efficient absorption in active layer.



[1] Finite Different Time Domain

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Figure1: schematic of simulated solar cell.

3D Simulation region boundary condition in x and y direction is Anti-symmetric and symmetric respectively. And PML[2] boundary condition in z direction has been chosen. A source in range of 300nm to 1100 nm that cover solar spectrum is illuminating as sunlight to the cell.

The absorption per unit volume, can be calculated from the divergence of the poynting vector as equation (2):

$$P_{abs} = -0.5\,\mathrm{Re}(\nabla.P) \qquad (2)$$

But, because divergence tend to more sensitivity in numerical problems, we can use more numerically stable formula as equation (3):

$$P_{abs} = -0.5\,\mathrm{Re}(i\omega E.D) \qquad (3)$$

Where shows dependence of the permittivity ε on the frequency ω.The photon energy at frequency ω is $\hbar\omega$, such that the number of photon absorbed per unit volume per unit time gives as equation (4):

$$g = \frac{P_{abs}}{\hbar\omega} = \frac{-0.5\left|E(r,\omega)\right|^2 \mathrm{Im}(\varepsilon(r,\omega))}{\hbar} \qquad (4)$$

In an ideal case we assume that all absorbed photons generate electron-hole pairs, so the photon-generation current will be written by equation (5):

$$I = q\int g(\lambda, r)dr \qquad (5)$$

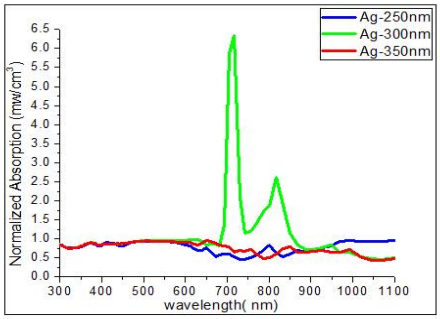
And for current density we would have:

$$J = \frac{I}{A} \qquad (6)$$

Where A refers to surface area of the cell.

3.results

At first we calculated normalized absorbed power (mw/cm^3) for three periods (distance of tow Nano rods centre) ,250 nm, 300nm and 350nm, that illustrated in figure (2) and figure (3) for silver and gold, respectively.



[2] Perfect Matched Layer

Figure2: absorption for three periods of 250nm, 300nm and 350nm for silver Nano rod in active region.

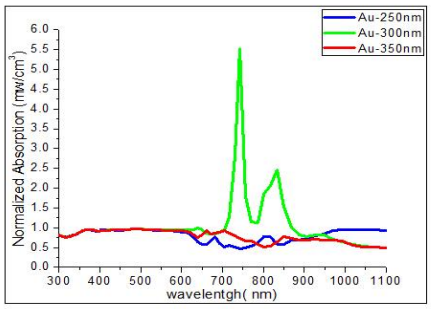


Figure3: absorption for three periods of 250nm, 300nm and 350nm for gold Nano rod in active region.

Just as defined in figures (2) and (3), absorption in 300 nm of periods is much more than others in both materials. This is due to that, in period of 250 nm the particles are very close to each other that led to more absorption in Nano rods, in both metals instead of active region. Also in period of 350 nm, due to the higher mode index, the absorption in other layers such as ITO and PEDOT: PSS is high, so we have high absorption in our transparent layers that decrease performance of the cell .

It is important to compare silver and gold metal for Nano rods, used in active region, to reach an optimum absorption in simulated solar cell.by incorporating silver and gold Nano rods with 150 nm thicknesses, 120 nm radiuses and 300 nm periodicity, absorption enchantment in active region studied, as shown in figure (4).

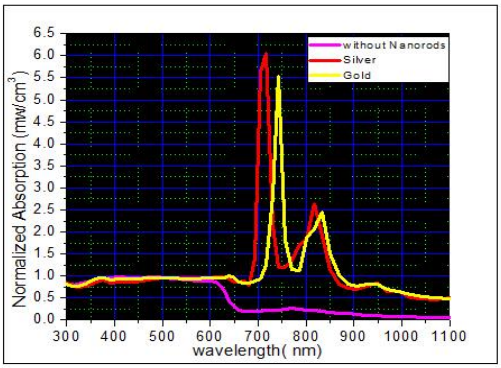


Figure 4: absorption by incorporating gold and silver Nano rods.

As shown in figure (4) without metal Nano rods, absorption will decrease mainly for wavelengths more than about 650 nm because the active region response is in this range due to its band gap energy. So for higher wavelengths (more than 650nm) and low energy of incident, we won't have excitation and electron-hole pairs

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generation, in active layer. By using metal nanoparticles, nanoparticles Fermi level will locate at sub-band gap region of active layer, so lower energy of incident light will absorb in active layer. so, the absorption will increase for high wavelengths in especially in resonance frequency (717nm and 816nm for silver and 743nm and 833nm for gold). Also, as shown in figure (5) the nearfield with metal Nano rods has increased in active region. Metal Nano rods embedded in active region as show in figure (5) have partially illuminated. Coupling This partially illuminating, and incident light, led to large scattering in active region that led to light path length enhancement in active layer, and so reason to enhance nearfield and more absorption in active layer. We also see that silver absorption peak is higher than gold. That is in agreement with calculation [10], refers to that the maximum light path length enhancement for silver is more than gold at Plasmon resonance frequency. Also we see that Ag and Au resonance wavelengths are very close to each other, because their real part of dielectric function, in near infrared range, is similar. But due to the imaginary part of the Au dielectric function, Au resonance has more red shifted than Ag.

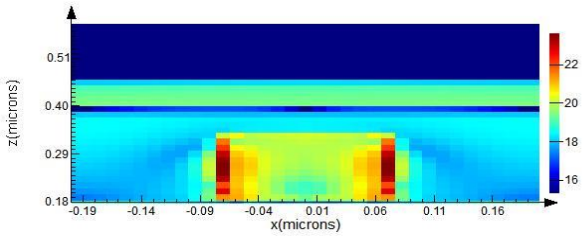


figure5: absorption of whole cell with Ag Nano rods in 717nm wavelength (at resonance peak).

4. Conclusion

We reached to high efficient absorption in P3HT: PCBM organic solar cell, by embedding noble metal, Ag and Au, Nano rods in active region. We reached to optimum parameters, radius 120 nm, height 150nm and period 300 nm, for Nano rods to high absorption purpose. High absorption has investigated by silver Nano rods at plasmonic resonance wavelength. In this simulation current density has increased perfectly from $19.10\,mA/cm^2$ to $52.66\,mA/cm^2$ and $49.75\,mA/cm^2$ with Ag and Au Nano rods respectively. That is great step for high absorption and current density in organic photovoltaic cells.

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