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Shape Effects on Light Absorption and Scattering for Nanoparticles in Thin Organic Films

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Abstract: A systematic study on the absorption enhancement by embedding metallic Nano Particles (NPs) in the Copper Phthalocyanine (CuPc) thin films has been reported. The Surface Plasmon resonance (SPR) can be excited by the addition of metal nano particles directly. Consequently, the incident light can be more focused and folded into the CuPc thin organic layers. The light scattering, and absorption have been applied on three shapes of silver nano particle (i.e. cylinder, hemisphere, and cross) by utilization of the Finite Different Time Domain (FDTD) software and the effect of change of NP size on the amount of light scattered and absorbed has been investigated. Finally, the effect of light absorption in organic solar cell performance upon embedding these metallic NPs directly into the organic CuPc thin films has been investigated.

Keywords*: *Nano Particles, Light Scattering and Absorption, FDTD Method

1. Introduction

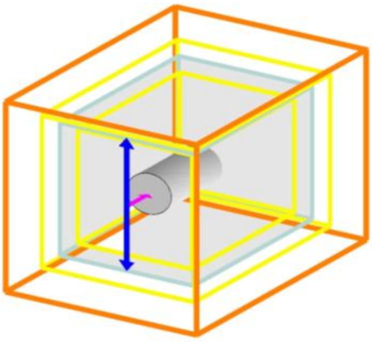
In the field of nanotechnology silver (Ag) and gold (Au), which are known as noble metal nanoparticles (MNPs), have played a vital role in the development of an extensive application in different fields such as photovoltaic cells (Kim *et al.*, 2015). A solar cell uses photovoltaic effect to convert the light energy of the sun into electricity (Dasri & Sompech, 2015). As an ideal alternative device, organic photovoltaic (OPV) cells have much potential as future-generation solar cells, because they are flexible, lightweight, and can be fabricated rather inexpensively (Baek *et al*., 2013). However, a major limitation of absorbance of light is ineffective in all thin film solar cell technologies (Kim *et al*., 2015). The enhanced optical absorption and short-circuit current have been theoretically and experimentally revealed in thin organic film solar cells by means of metallic nanoparticles (Qadir, Ahmad, & Sulaiman, 2014) which can be elucidated by the effects of plasmon-induced light-trapping and multiple scattering (Sha, Choy, Liu, & Cho Chew, 2011).

MNPs are able to scatter and absorb exciting incident visible light by the phenomenon of surface plasmon resonance (SPR). Plasmonic scattering from metal nanostructures has gained attention in various fields like surface enhanced Raman scattering (Abalde-Cela *et al*., 2010), evanescent-wave microscopy (Oheim, Loerke, Chow, & Stühmer, 1999), and other optoelectronic applications (Pillai *et al*., 2006). In the absorbing layers of photovoltaic cell devices, plasmonic scattering is intended to increase the absorption and offer efficient way to reduce its thickness. Experimentally, absorption enhancement has been studied from an integration of MNPs in different types of photovoltaic cells such as organic (Ihara, Kanno, & Inoue, 2010), dye-sensitized (Sha *et al*., 2011) , and amorphous silicon cells (Moulin *et al*., 2008). The great optical cross-sections and scattering efficiencies of localized surface plasmons (LSPs) are an ideal candidate to increase the ability of light trapping in photovoltaic cells (Atwater & Polman, 2010). The direction-dependent features of near-field scattering from NPs when embedded into the spacer are significantly affecting the enhancement of absorption (Sha *et al*., 2011).

This article focused on the enhancement of absorption by near-field scattering from NPs via Finite Difference-Time-Domain (FDTD) technique. The FDTD technique is the most common numerical method for solving a broad range of electromagnetic problems in a very accurate way (Troiani, Nikolic, & Constandinou, 2018). This technique consists of discretizing Maxwell's equations through the use of finite difference approximations for the derivatives (Nicolini & Bergmann, 2018). FDTD technique has been widely used in the past to study propagation near or through the ionosphere, and their extension to plasma devices such as antenna elements is a natural development (Nicolini & Bergmann, 2018), and is today's most popular technique which successfully applied to an extremely wide variety of problems, such as scattering from metal objects and dielectrics, antennas, microstrip circuits, and electromagnetic absorption in the human body exposed to radiation (Kunz, 2018). In this work, the absorption of visible electromagnetic field in the organic copper Phthalocyanine (CuPc) thin films have been simulated for different silver nanoparticles (Ag-NPs). Finally, the scattering and absorption spectra of various Ag-NPs using 3D full-field FDTD have been presented.

2. FDTD Simulation Model

The optical model is used to study the amount of scattered and absorbed light by Ag-NPs is depicted in the Figure 1. Absorbing boundary condition (PML) was used on the whole simulation side to avoid the effect of reflecting light. Total-Field Scattered-Field (TFSF) source is used to create a plane wave incident on MNPs. The light scattered by the NPs propagates beyond the TFSF boundary. Two power monitors are arranged and placed in two different regions: first in the total field and second in the scattered field region. In order to calculate the absorption coefficient and scattering cross sections, these monitors have been used. By means of this model, the absorption and scattering spectra of three Ag-NPs' shapes (cylinder, cross, and hemisphere) have been investigated.



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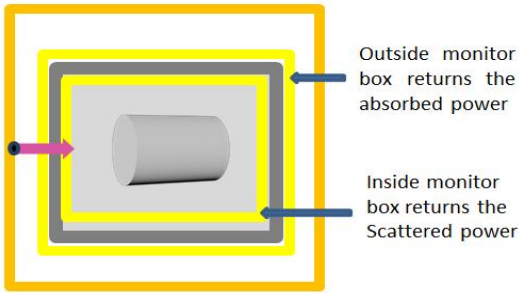

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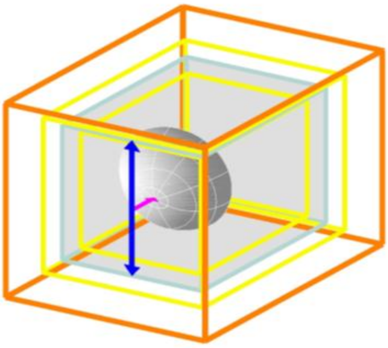

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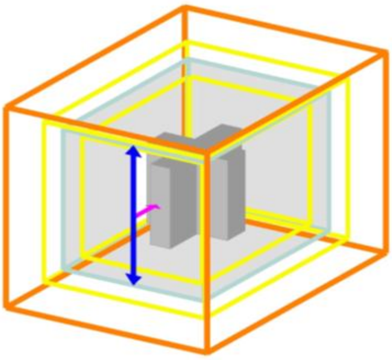
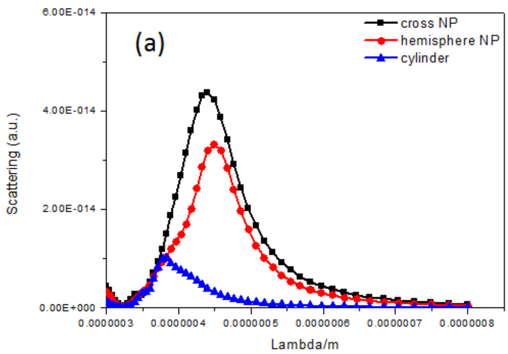


(d)

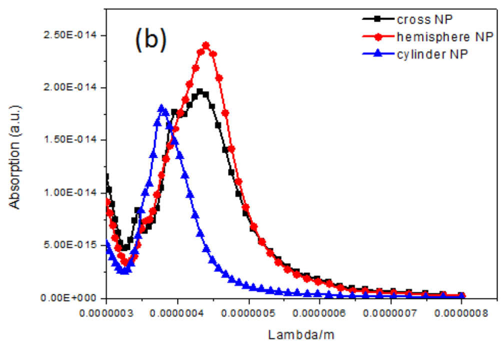
Figure 1: FDTD Model (a) cylinder Ag-NP (r = 30 nm, h = 60 nm), (b) side view of the model (a), (c) hemisphere Ag-NP (r = 50 nm), and (d) cross Ag-NP (w = 30 nm, x, y, z = 80 nm)

3. Result and Discussion

To investigate the effect of nanoparticle shape (NPS) on the amount of scattering light three various silver Ag-NPSs have been studied. As it is observed in the Figure 2 (a), different scattering spectra within the visible wavelength range is due to the effect of different Ag-NPs shape. In the case of the cross Ag-NP, the broadest and highest scattering spectra have been detected among three NPs. It is obvious in the wavelength range (3×10^{-7}- 8×10^{-7} m) of the Figure 2 (b) that different Ag-NPs have different absorption spectra. Shape alteration in the particles (from hemisphere to cross and cylinder) led to a reduction of the absorption spectra respectively.



(a)

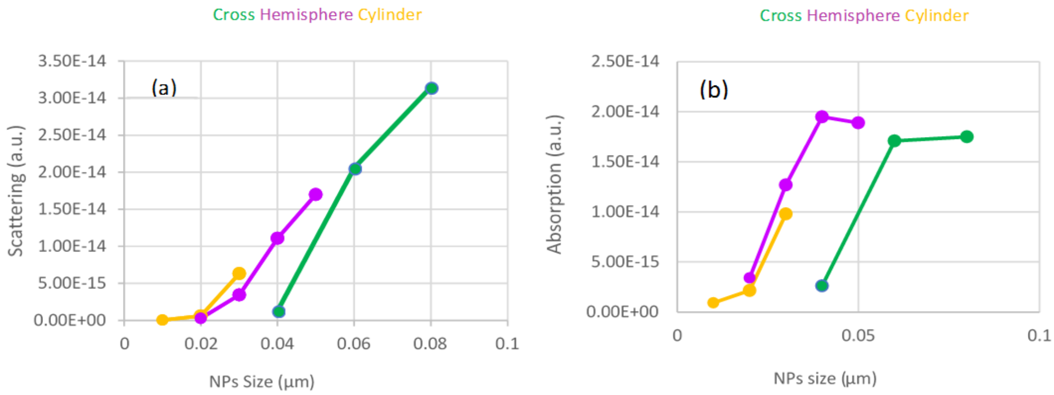


(b)

Figure 2: (a) Light scattering spectra and (b) Light absorption spectra of different Ag-NP shapes

The effect of the NPs size on the amount of scattering and absorbing light is the second step of this investigation (depicted in the Figure 3 (a) and b). In the case of hemisphere Ag-NPs, increasing the radius (r) from 20 nm to 30, 40, and 50 nm lead to increase the scattering pick from 0 to 4×10^{-15}, 1.18×10^{-14}, and 1.75×10^{-14} respectively in the specific wavelength of 4.51×10^{-7} m. Changing the size of cross Ag-NP from width w = 10 nm and x, y, z = 40 nm to width w = 20 nm and x, y, z = 60 nm; and to width w = 30 nm and x, y, z = 80 nm lead to increase scattering pick from 1×10^{-15} to 2×10^{-14} and 3.2×10^{-14} in the wavelength of 4.5×10^{-7} m.

For cylinder Ag-NP decreasing radius from 30 nm to 20 and 10 nm, and high h from 60 nm to 40 and 20 respectively lead to reduce scattering pick from 5.2×10^{-15} to 1×10^{-15} and then 0 respectively in the wavelength 3.8×10^{-7}m. In the same manner the absorption pick (as shown in the Figure 3 (b)) in the wavelengths 4.4×10^{-7}, 4.3×10^{-7} and 3.7×10^{-7} m for the hemisphere, cross, and cylinder shapes of Ag-NP respectively are changed by changing Ag-NP sizes. The data obtained from the simulations, compared with the experimental results from reference (Shamjid *et al.*, 2017), the experimental results might be in close agreement with the theoretical simulations in present work.



(a) (b)

Figure 3: The effect of change of NPs size on the amount of light (a) Scattering (b) Absorption

In order to study the effect of scattering by NPs on the absorption efficiency, similar shapes (cross, cylinder, and hemisphere) have also been utilized to investigate the effect of scattering on the absorption in thin organic films. The software of Lumerical FDTD solutions has been used for different NPs to exploit the ultimate potential efficiency. FDTD is used to calculate how the electromagnetic fields propagate from the source through the structure. Subsequent iteration results in the electromagnetic field propagation in time. Typically, the simulation runs until there is no electromagnetic fields left in the simulation region.

It's worth noting that, Copper Phthalocyanine (CuPc) (Qadir *et al.*, 2014) as one of the most common materials of organic solar cell has been employed with 80 nm thickness. Same Ag-NPs have been chosen to embed inside CuPc thin organic films. The absorption spectra in CuPc thin film without and with metallic shapes of cross, cylinder, and hemisphere NPs is depicted in the Figure 4. Compared the absorption spectra of the pristine CuPc thin organic film, CuPc thin organic films with metallic NPs are significantly enhanced. The observed improvement in the wavelength range 35–55 nm is worth a closer look. Moreover, it is evident that the different absorption enhancement due to the effect of different Ag-NPs can be achieved. Similarly, it is noticed before that different Ag-NPs have different scattering spectra. CuPc with change in the shape of Ag-NPs from the cross to hemisphere, then cylinder led to the absorption reduction in organic CuPc thin film. The reason is due to the reduction of multiple scattering spectra for the hemisphere and cylinder as it is observed in the previous result the Figure 2 (a). As the comparison of the figures 2 (a) and 4 showed that among these three shapes cross shape Ag-NPs has proved itself as the broad scattering spectra and best shape to improve absorption enhancement in CuPc thin organic film. However, cylinder NPs have lowest scattering spectra consequently lowest absorption enhancement effect on CuPc thin organic film. Regarding to the reference (Schmid, Andrae, & Manley, 2014) the light scattered by nanoparticle plays a key role to enhance the absorption in CuPc thin film.

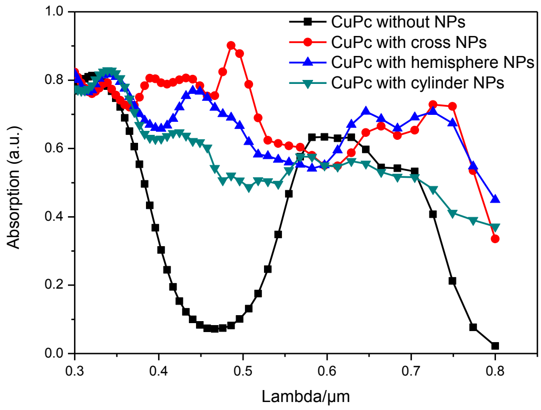


Figure 4: The absorption enhancement in CuPc thin organic films based on the effect of NPs shape

4. Conclusions

In this study, the Ag nanoparticles were prepared by the FDTD technique which is extremely useful for improving performance without using chemicals. We numerically investigated the light scattering properties of Ag nanoparticles with various sizes and shapes. The absorption spectra of the various Ag-NPs were studied. The absorption properties of a few Ag-NPs embedded in the thin organic films were presented using FDTD optical simulation. The effects of metallic NPs size on the amount of light scattered and absorbed were also presented. The results show that the NPs' shapes and sizes have the potential effects on the visible light scattering and absorption enhancement in CuPc thin films.

Acknowledgement

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