

A theoretical analysis of plasmonic effects of metallic nanoparticles in organic solar cells

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A theoretical analysis about the influence of metallic nanoparticles embedding in organic solar cell has been developed. An algorithm based on the finite difference frequency domain (FDFD) method has been used. The algorithm leads to observe that the size of metallic nanoparticles enhances in different wavelength the optical electric field.

Keywords—Organic solar cell, plasmon effect, trapping light, metallic nanoparticles.

I. INTRODUCTION

Organic solar cells (OSCs) are devices of third generation which present many advantages over other solar cells such as flexibility, lightweight and unique condition: transparency. But also, present disadvantages such as their low power conversion efficiency (PCE) and short lifetime. One proposal to improve the PCE is to increase the light absorption by embedding metallic nanoparticles into the active layer (P3HT:PCBM) to generate a phenomenon called surface plasmon resonance. Recently, several works have reported the used of nanoparticles to increase the power conversion efficiency, it has been proposed that the size, shape or distribution of nanoparticles in the active layer have effects on the light absorption of metallic nanoparticles [1] [2].

In this work, a theoretical analysis of the optical electric field in an active layer of OSCs with embedded metallic nanoparticles is presented. By using the Finite Difference Frequency Domain (FDFD) method, the Helmholtz wave equation in the frequency domain was solved.

II. BASIC EQUATIONS AND SOLUTION METHOD

A. Basic Equations

Starting from Maxwell's equations and using the vector identity $\nabla \times \nabla \times \mathbf{A} = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}$, we can obtain the Helmholtz wave equation in the frequency domain:

$$\nabla^2 \mathbf{E}_s - \gamma^2 \mathbf{E}_s = 0, \quad (1)$$

where, $\gamma^2 = j\omega\mu\sigma - \omega^2\mu\varepsilon$ is the propagation constant, in which ε is the electric permittivity, ω is the angular frequency, σ is the conductivity and μ magnetic permeability.

If we consider that the electromagnetic wave propagates in the $-z$ -direction and that we are interested in calculating the optical electric field in the zx -plane, the equation (1) can be written as:

$$\frac{\partial^2 \mathbf{E}_s}{\partial x^2} + \frac{\partial^2 \mathbf{E}_s}{\partial z^2} - \gamma^2 \mathbf{E}_s = 0. \quad (2)$$

B. Algorithm Development

The active layer was discretized in space using n nodes for z -direction and m nodes for x -direction. Fig. 1. Each node represents a point where the electric field is calculated. Dirichlet condition was used at the border where the electromagnetic radiation gets in and Neumann conditions were used in the other borders.

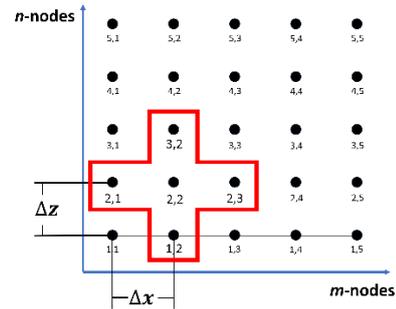


Fig. 1. Discretization of the active layer.

C. Finite Difference Approximation

To calculate the electric field, the equation (1) was discretized by approximating the differential equation derivative by finite differences,

$$\frac{df(x_0)}{dx} \approx \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}. \quad (3)$$

The Helmholtz equation, put into discrete form, can be expressed as:

$$\frac{\mathbf{E}_{i+1,j} - 2\mathbf{E}_{i,j} + \mathbf{E}_{i-1,j}}{(\Delta x)^2} + \frac{\mathbf{E}_{i,j+1} - 2\mathbf{E}_{i,j} + \mathbf{E}_{i,j-1}}{(\Delta z)^2} - \gamma_{i,j} \mathbf{E}_{i,j} = 0, \quad (4)$$

where, $i = 1, 2, \dots, n$ and $j = 1, 2, \dots, m$.

III. RESULTS

A. Wave Propagation in a stratified Medium

To validate the algorithm, we calculate the electric field inside of an OSC structure, Fig. 2, reported in the literature [3], which is a stratified medium. For this case, refractive index (n) and extinction coefficient (k) for each material was used to obtain the corresponding parameters: ϵ , σ and μ . The result at a wavelength of 600 nm, Fig. 3a, was compared with the optical electric field obtained by the transfer-matrix method in one dimension, Fig. 3b. From these figures, we can observe that both results are similar.

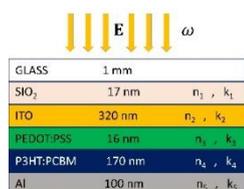


Fig. 2. The incident light radiation in a stratified organic solar cell.

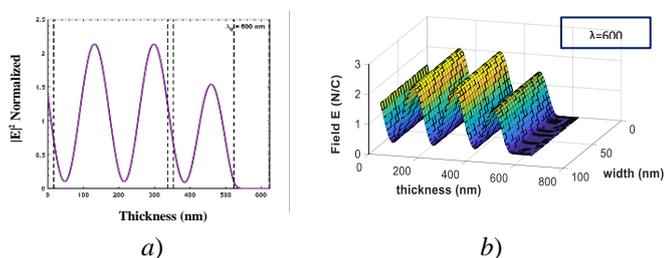


Fig. 3. Optical electric field inside the OSC structure calculated by a) the transfer matrix method and b) the numerical solution in two dimensions.

B. Wave Propagation in a Single Medium with Nanoparticles

To analyze the effect of the metallic nanoparticles on the optical electric field, we consider the P3HT:PCBM system as an active layer with and without gold nanoparticles in a film 100 nm thick, Fig. 4. The wavelength of the electromagnetic radiation was 600 nm. From Fig. 5, we can observe the increase of electric field when the nanoparticles are embedded.

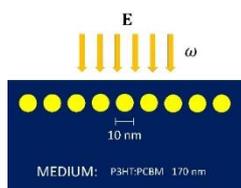


Fig. 4. The incident light in a mixed medium with nanoparticles.

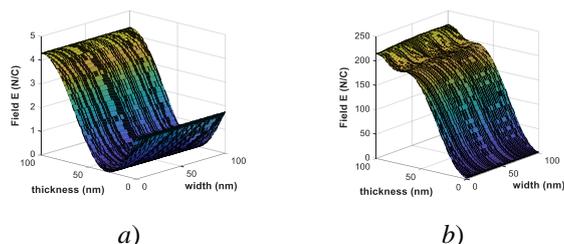


Fig. 5. Optical electric field inside the active layer of an OSC a) without nanoparticles and b) with nanoparticles.

C. Electric field for different size of nanoparticles

To analyze the plasmonic effect, we calculated the double integral of the optical electric field as a function of the wavelength, in the spectral range of 300-900 nm, for three nanoparticle sizes: 5nm, 10 nm and 15nm,

$$f(\lambda) = \int_0^d \int_0^w E(x, z, \lambda) dx dz. \quad (5)$$

It should be noted from Fig. 8, that each curve has a peak, which can be related with the plasmonic effect.

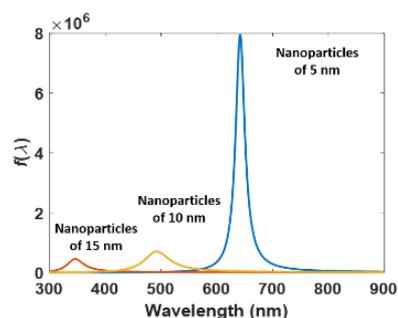


Fig. 8. Integral of the optical electric field as a function of the wavelength for three different nanoparticle sizes.

IV. CONCLUSION

The algorithm leads to observe that the size of metallic nanoparticles enhances in different wavelength the optical electric field. It is inferred that such a behavior is related with the influence of plasmonic effect when using metallic nanoparticles in the active layer of organic solar cells.

ACKNOWLEDGMENT

The authors would like to thank financial support from Instituto Politécnico Nacional (project sip 20195536) and Consejo Nacional de Ciencia y Tecnología - CONACYT.

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