3D Modeling and optimization of Organic Solar Cells

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Abstract - In this paper a new design process for Organic Solar Cells (OSCs) are proposed and developed using the commercial modeling software for technical design and a simulation tool Comsol vers. 5.3. Comsol was used to determine the electromagnetic fields on OSCs element interfaces and to optimize aluminum and active layers. A more efficient geometry was founded in order to maximize the light trapping and increase the photovoltaic market. The first experimental results on the new OSCs are reported.

Keywords: Industrial lime, treatment, pollution, energy recovery,environment, distillation

I. INTRODUCTION

The third-generation solar cells can be made of low-cost and sustainable materials such as polymers however with less efficiency than the standard silicon cells mainly limited by the ability of the active layer to absorb light and convert it into electricity. A good solution could be investigate new light trapping techniques and the impact of geometry in new model and architecture design [1]. In organic solar cells (OSCs) the geometrical parameters influence significantly the efficiency and performance. The variation in the length of the devices is not negligible affecting the recombination of charge carriers in the organic solar cells. Many authors have demonstrated as the geometry of organic solar cells influences the electrical enhancements, the absorption and scattering efficiency of the particles [2-8]. The authors in describe the effect of geometrical parameters, particularly shape, on optical absorption enhancement for thin film solar cells based on crystalline silicon (c- Si) and gallium arsenide (GaAs) using a rigorous coupled wave analysis (RCWA) method. The light trapping schemes for organic thin film solar cells include geometric engineering of the structure of the solar cell at the micro and nanoscale, plasmonic structures, and more as reported in [4].

For specific types of geometrically shaped solar panels a simpler method was derived and applied, however with the limitations to broaden the applicability of the model to a wider range of geometric shapes.

Deepak K. Gupta et al present an efficient manner to maximize the power output with the application of topology optimization (TO) to optimize the front metallization patterns for free-form solar cells that are cells of unconventional shapes (e.g. hexagonal, leaf-shaped, circular, motorbike fairings etc) with flexible shape added to the aesthetics of the surround- ings and an important factors of metallization design [8]. In order to provide more absorbtion of solar radition graphene nanostructures are incorporates from 0.5 to 5 µm in the device design or reduced graphene oxide as anode buffer layer is used. Graphene has a high optical transmittance, an excellent electron/hole transport properties, superior mechanical stiffness and flexibility. The Graphene can be used as transparent electrode to retard charge recombination in OPVs .To reduce or retard the carrier recombination we could form a direct channel between anode and cathode creating an alternating of graphene and ITO patterns. Other authors have investigate the electromagnetic field induced on solar devices in order to evaluate the interactions of the optical model at several frequencies and the magnetic field using as tool COMSOL to calculate the electric field effects starting from an organic sample. In this work we have presented different three-dimensional models of multilayer bulk hetero- junction organic nanoscale solar cells. The 3D simulations of electromagnetic fields applied to OSCs presented in this work clearly reveal that the physical mechanisms depend on this particular contact design [9]. Using a cross-platform finite element analysis, solver and Multiphysics simulation software, we have analyzed specific geometrical patterns that could be optimal for capturing and holding light in thin-cell organic solar cells.

II. GEOMETRIC MODEL

A solar organic cell is schematized in Fig. 1. In order to investigate the shape in OSCs we proposed new design with different geometry types that could lead to more efficient organic solar cells. Five main parts are assembled in the electronic device such as a rigid glass support, an anode, an intermediate layer, a photo-active layer and cathode layer [8]. The glass support has the peculiarity to be transparent for light. Furthermore, Indium Tin Oxide (ITO)is used as anode or positive electrode with a work function greater than metal [3]. The intermediate layer consists of conductive polymer PEDOT: PSS (Poly (3,4 ethylenedioxythiophene) poly (styrenesulfonate)) layer deposited directly on anode with the Spin-coater 2.The active material is deposited on PEDOT:PSS layer mainly composed of poly (3-hexylthiophene) (P3HT) and the fullerene (6,6)- phenyl-C61 butyric acid methyl ester (PCBM) responsible for light absorption, charge carrier production, and carrier separation. Aluminum is evaporated used exclusively as cathode.

The parametric modeling of the OSCs was performed in a similar way to that described by Calì et al. [10,11].

The parametric 3D design software of Solidworks has been an useful tool to model mechanical and electronic device.

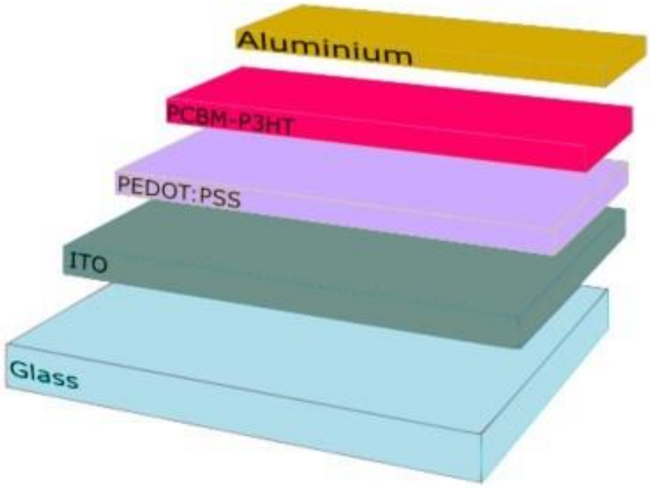

Fig. 1. OSC structure

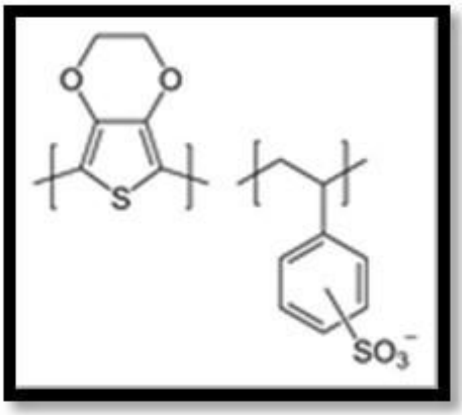

Fig. 2. PEDOT:PSS structure

In our case we have considered the device manufactured (Fig.4) in the laboratories in the University of Ben Gurion [1], [5]. The thickness of ITO is 70 nm on 0.7 mm thick glass substrate (12 × 12 mm), 30 nm of PEDOT: PSS, 200nm the P3HT:PCBM and 90 nm aluminum cathode. In each sample are inserted four OSCs with different lengths 7.5, 6.5, 5.5 and 4.5 mm. Rendering and 3D visualization problems are avoid increasing the thickness of deposited materials and decreasing the size glass thickness as in Fig. 3. On the basis of OSCs structure, different alternative shapes are proposed for aluminum cathode taking in account the increasing of charge density. The electrons and holes inside the metal react to the electromagnetic excitation inducing surface charges. The local surface charge density increases drastically in geometrical singularity such as tip apex. We have investigated the effects of different geometry characterized of several tip apexes to response to electromagnetic excitations. In general, the charge density is concentrated in the region with largest value of curvature and thus smaller radius of curvature. Two charged spherical conductors of radius R1 and R2 with R2 > R1 connected by a conducting wire. The potentials V1 e V2 have to be the same, the charge on each sphere is in proportion to their radii:

$$V_1 = V_2 = \frac{1}{4\pi\varepsilon_0}\frac{Q_1}{R_1} = \frac{1}{4\pi\varepsilon_0}\frac{Q_2}{R_2} \qquad (1)$$

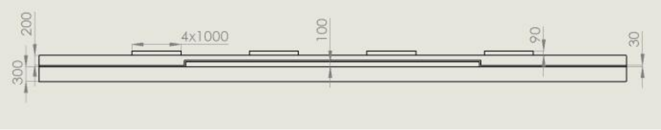

Fig. 3. OSC side view

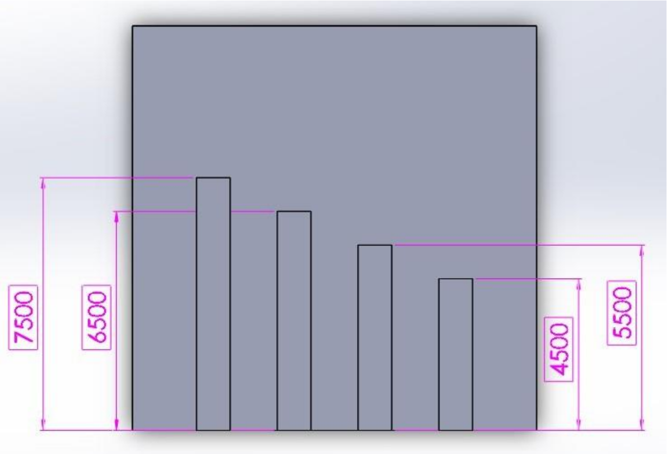

Fig. 4. Modelled OSC structures

The final charges are then:

$$\frac{Q_1}{R_1} = \frac{Q_2}{R_2} = cost = K \qquad (2)$$

This means that the surface charge density of the smaller sphere is larger, i.e. that the charge is more crowded per unit area on the smaller sphere.In particular the ratio between the charge density Q on the surface of the sphere and the radius R is constant and with the same potential. For smaller surface namely largest curvature, lower surface charge density distribution is observed than larger surface.

The surface charge densities are calculated:

$$\sigma_1 \frac{Q_1}{4\pi R_1^2} \qquad (3)$$

$$\sigma_2 \frac{Q_2}{4\pi R_2^2} \qquad (4)$$

as resulted:

$$\sigma_1 \frac{K}{4\pi R_1^2} \qquad (5)$$

$$\sigma_2 \frac{K}{4\pi R_2^2} \tag{6}$$

The surface charge density is lower on second sphere. Thus the curvatures and apertures of the tip apex strongly influence the density charges. The effects of different apertures, curvature and sharpness of tip are analyzed to enhance the efficiency and electromagnetic field in OSCs. To model the cell with the rectangular cathode a 2D sketch was created on the upper face of the active layer and using the ”rectangle of the corner” function, it was possible to draw the cathodes. Through the “basic extrusion” function, it was possible to realize the final form. To create the Arabic cell, a 2D sketch was created on the upper face of the active layer 5. Using the ”spline” function, it was possible to draw the curved profile of the cathode.

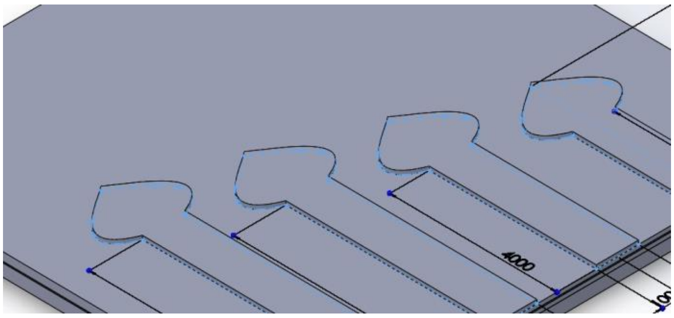

Fig. 5. Model of OSCs inspired to Arabic style

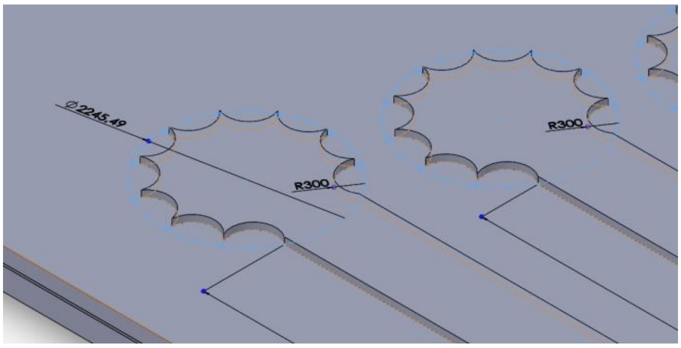

Fig. 6. Model of OSCs inspired to nine-pointed stars

The rectangular part was created using the ”rectangle of the corner” function. Extruding the sketch the shape of an Arabic shape was created. The nine-pointed star shape was also created by a 2D sketch on the upper face of the active layer12. First a circumference with a radius equal to 2245 µm was drawn using the ”circle” function, then another circle with a radius of 300 µm and a geometric center on the first circumference was drawn. First of all using the ”circular repetition” function and then the ”shorten entities” function, it was possible to obtain the definitive profile The pentagonal shape was configured by means a 2D sketch on the upper face of active layer 6. Using the ”polygon” function a hexagon has been created inscribed in a circumference having a diameter equal to 1376 µm, with the ”tangent arc” function it was possible to realize the curved shape of the sides as shown in Fig. 7.

III. Simulation Model

The types of geometric models proposed of the samples processed in SolidWorks have been imported in COMSOL and then the physical parameters has been set useful for the simulation of electromagnetic field. We have considered the Maxwell equations with particular referring to the electric field E and the magnetic flux density B as reported below:

$$\nabla \cdot \mathrm{E} = 0 \tag{7}$$

$$\nabla \times \mathrm{E} = -\frac{\partial B}{\partial t} \tag{8}$$

$$\nabla \cdot \mathrm{B} = 0 \tag{9}$$

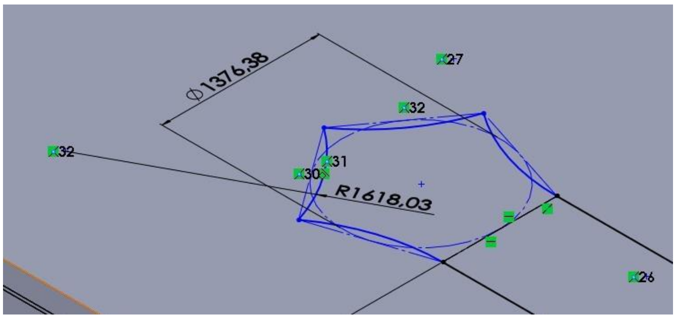

Fig. 7. Model of OSCs inspired to pentagon shape

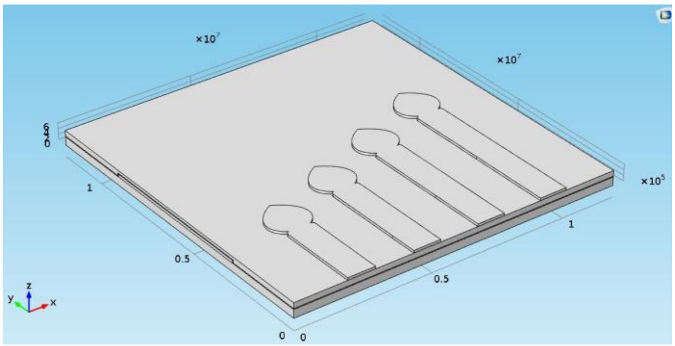

Fig. 8. Arabian style model

$$\nabla \times \mathrm{E} = \mu\varepsilon \frac{\partial E}{\partial t} \tag{10}$$

The material properties are described using relative permeability ε and the relative permittivity μ. In this application RF module is used for Multiphysics simulation models for wavelengths of the visible spectrum from 400 nm to 700 nm. In order to guarantee the simulation phenomena, optical values and electric properties of different materials are used as reported in [2]. Each sample was exposed to an incident light beam. Considering the discretization by Finite Element Method in order to obtain reliable simulation results, was used “Free mesh” able to automatically thicken free elements on the edges of the organic cell. On the basis of the light incident on device, the electromagnetic field is applied in perpendicular direction on glass substrate chosen as active port for port boundary conditions. The outgoing signal is determined on surface of the aluminum cathode whereby to calculate the electric field, the magnetic field and power electric flow. From obtained results, power electric flow for cathode of 5.5 mm has less electric value considering rectangular shape aluminum than pentagonal shape as reported in Fig. 9.The maximum peak of electric field along the direction of the organic cell is obtained for length of 5.5 mm and has a value of $2.91*10^{-4}$ Vm^{-1}.

IV. CONCLUSIONS

In this paper the ultrathin organic solar cells costitued by GLASS/ITO/PEDOT: PSS/ PF3HT:PCBM/ Al layers with different geometry of aluminum cathode are investigated. In particular different geometrical models of OSCs are proposed using the 3D design software SolidWorks and processed in COMSOL to simulate the physical phenomena of electromagnetic fields.

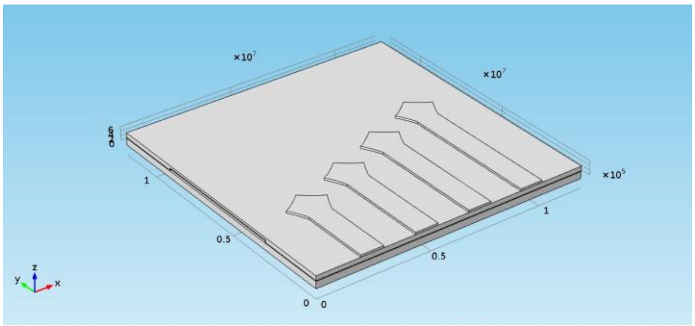

Fig. 9. Pentagonal style model

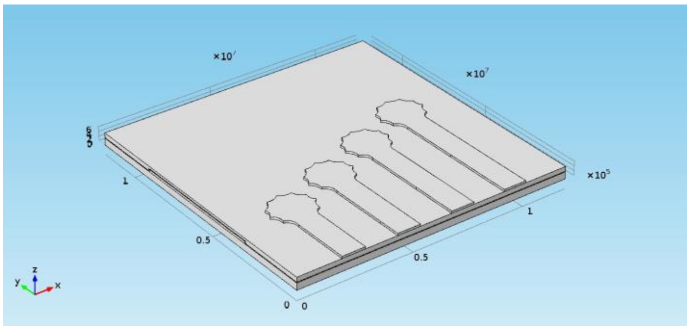

Fig. 10. Star style model

The proposed shape of Aluminum cathode are rectangular, pentagonal and nine-pointed stars and are simulated using the RF Module of Comsol Multiphysics. The optimal results of electric field are obtained for cathode of 5.5 mm with pentagonal shape. Thus we have demonstrated that the shape of cathode influences the performances of solar cells.

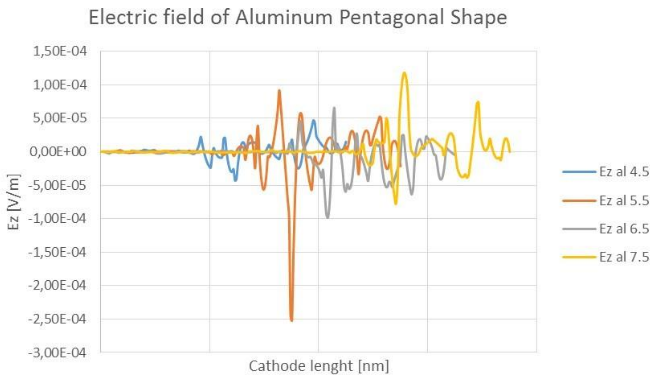

Fig. 11. Electric Field Aluminum pentagonal Shape

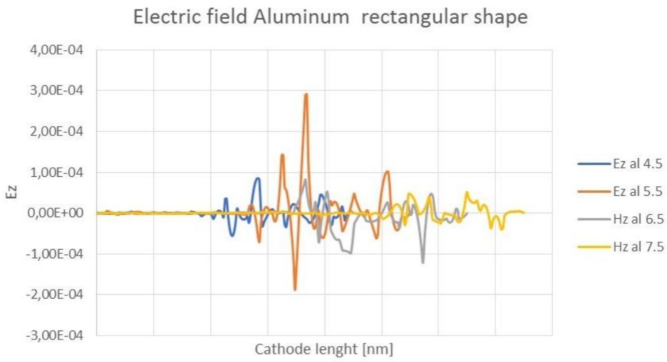

Fig. 12. Electric Field Aluminum rectangular Shape

In our case based on charge density distribution it is observed that for lower curvature of Aluminum cathode the electric field increases also for lenght dimensions of 5.5 nm.

REFERENCES

[1] F. Bonanno, G. Capizzi, and C. Napoli. Some remarks on the application of RNN and PRNN for the charge-discharge simulation of advanced Lithium-ions battery energy storage. In Power Electronics, Electrical Drives, Automation and Motion , pp.941-945. 2012.

[2] G. Capizzi, G. Lo Sciuto, C. Napoli, and E. Tramontana. A multithread nested neural network architecture to model surface plasmon polaritons propagation. Micromachines, 7(7), 2016.

Yen-Ju Cheng, Sheng-Hsiung Yang, and Chain-Shu Hsu. Synthesis of conjugated polymers for organic solar cell applications. Chemical reviews, 109(11):5868–5923, 2009.

[3] WI Nam, YJ Yoo, and YM Song. Geometrical shape design of nanopho- tonic surfaces for thin film solar cells. Optics Express, 24(14):A1033– A1044, 2016.

[4] G. Capizzi, G. Lo Sciuto, C. Napoli, R. Shikler, and M. Woźniak. Optimizing the Organic Solar Cell Manufacturing Process by Means of

AFM Measurements and Neural Networks. Energies, 11(5), pp.1-13. 2018.

[5] G. Lo Sciuto, G. Capizzi, C. Napoli, R. Shikler, D. Połap, and M. Woźniak. Exploiting OSC Models by Using Neural Networks with an Innovative Pruning Algorithm. In International Conference on Artificial Intelligence and Soft Computing, pp. 711-722. Springer. 2018.

[6] Sean E Shaheen, Christoph J Brabec, N Serdar Sariciftci, Franz Padinger, Thomas Fromherz, and Jan C Hummelen. 2.5% efficient organic plastic solar cells. Applied Physics Letters, 78(6):841–843, 2001.

[7] Holger Spanggaard and Frederik C Krebs. A brief history of the development of organic and polymeric photovoltaics. Solar Energy Materials and Solar Cells, 83(2-3):125–146, 2004.

[8] Calì, M., Oliveri, S. M., Sequenzia, G., & Fatuzzo, G. (2017). An effective model for the sliding contact forces in a multibody environment. In Advances on Mechanics, Design Engineering and Manufacturing (pp. 675-685). Springer, Cham.

[9] Calì, M., Zanetti, E. M., Oliveri, S. M., Asero, R., Ciaramella, S., Martorelli, M., & Bignardi, C. (2018). Influence of thread shape and inclination on the biomechanical behaviour of plateau implant systems. Dental Materials, 34(3), 460-469.

[10] Calì M., Oliveri S. M., Ambu R., & Fichera G. (2018). An Integrated Approach to Characterize the Dynamic Behaviour of a Mechanical Chain Tensioner by Functional Tolerancing. Strojniski Vestnik/Journal of Mechanical Engineering, 64(4). doi:10.5545/sv-jme.2017.5079