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Finite Element Modeling of Bilayer P3HT/C60 Organic Solar Cells: Influence of Active-Layer Thickness on Optical Performance

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INTRODUCTION & AIM

Polymer–fullerene organic solar cells (OSCs) are attractive for their low cost, mechanical flexibility, and compatibility with large-area fabrication. Bilayer architectures using poly(3-hexylthiophene) (P3HT) as the donor and fullerene (C60) as the acceptor provide a simple geometry with well-defined donor–acceptor interfaces. However, their performance is highly dependent on the optimization of active-layer thicknesses to balance light absorption and charge generation. [1].

To model and analyze the optical behavior of bilayer P3HT/C60 organic solar cells using FEM simulations, aiming to optimize the active-layer geometry for improved light absorption and charge generation efficiency. A Finite Element Method (FEM) model implemented in COMSOL Multiphysics is used to calculate:

- The spatial distribution of the electric field, the photon absorption generation rate, and the reflectance behavior.
- The obtained exciton generation rate (G) allows identifying the optimal conditions for achieving higher optical efficiency of the cell.

METHOD

Two-dimensional optical simulations were conducted using the finite element method (FEM) to analyze a bilayer OSC stack composed of a glass substrate, a SiO_2 buffer layer, an indium tin oxide (ITO) anode, a PEDOT:PSS hole transport layer, a P3HT/C60 active region, a lithium fluoride (LiF) electron transport layer, and an aluminum (Al) cathode. The optical field distribution and exciton generation rate (G) were evaluated under monochromatic illumination at incident wavelengths of 350, 530, 740, and 860 nm, as well as under the AM1.5G solar spectrum at 100 mW/cm².

Optical Model [1-3]

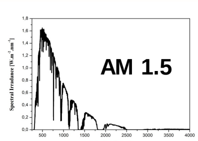
COMSOL MULTIPHYSICS®

Dissipated energy (W.m-2 nm-1)

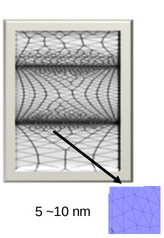
$$\varphi(z,\lambda) = \alpha(\lambda)\frac{n_i}{n_0} I_{solar} \left|\frac{E(z)}{E_0}\right|^2$$

$$G(z,\lambda) = \frac{\varphi(z,\lambda)}{\hbar\upsilon}$$

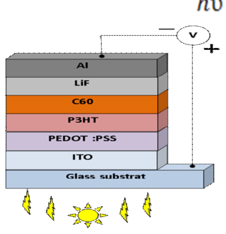
$$G(z) = \sum_{\lambda=300}^{900} G(z,\lambda)$$



The incident light

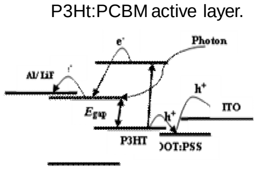


Mesh of the studied structure (FEM)



The incident light

The Energy potential diagram P3Ht:PCBM active layer.



RESULTS & DISCUSSION

Figure 1: **Electric field intensity** versus cell depth (nm) in the optimized P3HT/C60 active layer solar cell.

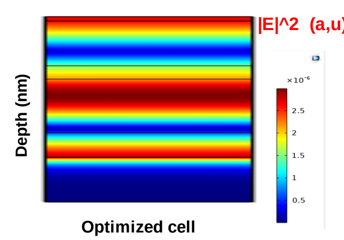


Figure 2: Total **energy dissipation** power density of the optimized cell as a function of the P3HT/C60 active layer solar cell.

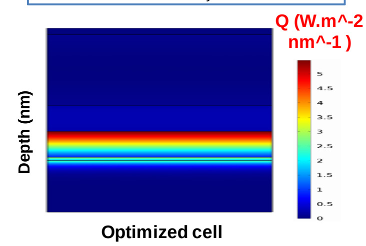


Figure 3: Calculated **electric field intensity** as a function of the P3HT/C60 cell depth in the unoptimized and optimized devices (nm).

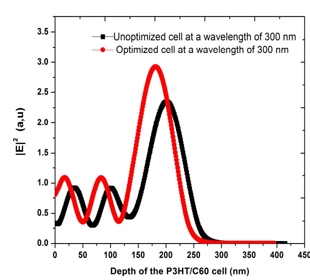


Figure 4: Calculated **generation rate** as a function of the P3HT/C60 layer depth (nm) in the unoptimized and optimized devices.

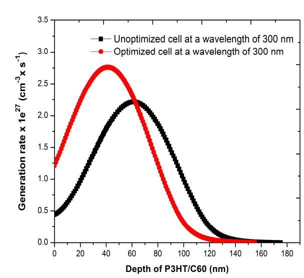


Figure 5: Calculated reflectance of the device for the optimized cell.

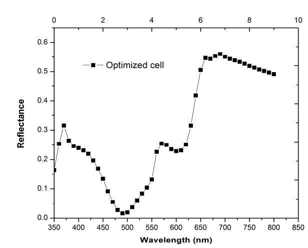
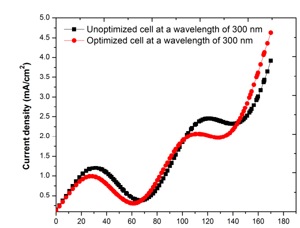


Figure 6: Calculated short circuit current density in the unoptimized and optimized devices.



CONCLUSION

* The spectral response and active-layer thickness strongly influence device performance.
* Distinct resonance patterns appear at specific wavelengths, enhancing exciton generation within the absorber.
* Optimal light confinement and balanced charge generation are achieved for a 100 nm P3HT layer with a 55 nm C60 layer.

• Finite element simulations using COMSOL Multiphysics strongly correlated with experimental data, validating the design's effectiveness in optimizing performance.

FUTURE WORK / REFERENCES

Future work will focus on Incorporation of optical management layers (OMLs), nanostructures, or back reflectors improves spectral capture and spatial distribution of the optical field.

[1] Brioua, F., Remram, M., Nechache, R., et al. **Appl. Phys. A**, 123, 704 (2017).
[2] Brioua, F., Daoudi, C., Mekimah, B., Lekouaghet, B. **Phys. Scr.**, 99, 085951 (2024)
[3] Fathi, B., Chouaib, D. **Iran. J. Mater. Sci.**, 21(2), 1 (2024).