# Optimization of $MAPbI_3$ Perovskite Solar Cell with Nano Structures

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***Abstract*—Perovskite solar cell has been a promising low cost high efficiency solar cell and the efficiency increase rapidly. Since the crystal quality issues have been improved significantly, a further numerical optimization in the structure design is needed. We applied FDTD program for optical absorption and use our Poisson and drift-diffusion solver for electrical simulation. The Poisson and drift-diffusion solver is optimized for sovling organic and inorganic materials. Finally, we design a nano-structure that have efficiency of $MAPBI_3$ based solar cell has been improved from 18% to 19.67% That efficiency has be enhanced by 12% compared to the planar structure.**

***Index Terms*—2D-Drift-Diffusion, 2D-FDTD, Perovskite, Solar cells, $MAPBI_3$, Organic**

## I. Introduction

Recent studies showed that the power conversion efficiency of perovskite based solar cell has been improved from 3.8% to more than 20% in a few years. Hence, perovskite material based solar cells have attracted significant attention for researchers to work on this material. Generally, perovskite has some advantages, such as it have a higher absorption coefficient. It can be fabricated by low-cost material and process and it can be designed to grow on flexible substrate as a flexible solar cell. However, not many works are done by a complete numerical model to investigate the electrical properties of the perovskite solar cells, which is critical and essential for optimizing the overall performance of solar cells. In this paper, the optical properties and electrical properties of $MAPBI_3$ solar cells are investigated and analysed. And the content is organized as followings: (1) We will first show you the device structure for simulation; (2) then the methodology for simulating the $MAPBI_3$ based solar cells; (3) the simulated results are presented and discussed as well as the optimization methods are proposed.

## II. Methodology

### A. Simulation of optical field

Our lab has established the two-dimensional finite-difference time-domain (2D-FDTD) method for optical simulation of solar devices. The 2D-FDTD program can be used calculate wave distribution in the layer of solar cells even with arbitrary nano structures. The 2D-FDTD method has been built by Maxwells equations with discrete space and time dimension.

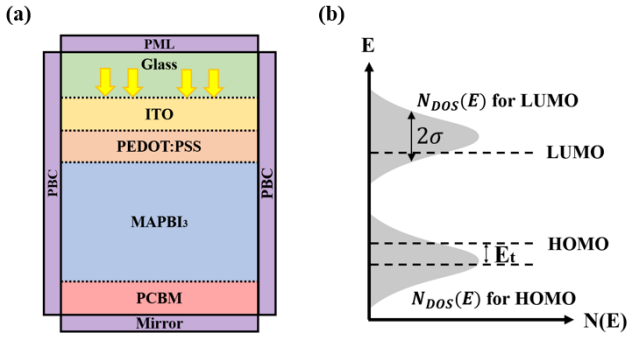


Fig. 1. (a) The simulated structure with 2D-FDTD optical solver; (b) The Gaussian-like density of states.

The boundary condition on top of the device is perfectly matched layer (PML) to prevent the reflection from the upper layer. In x-direction is periodic boundary condition (PBC) since the planar perovskite solar cells are periodic in x-direction. At the bottom of the device, perfect electrical conductor (PEC) is used to present the condition of metal electrode reflecting back the light. Fig.1(a) show the boundaries of this simulation.

### B. Simulation of electrical properties

The two-dimensional finite element method (FEM) Poisson′s and drift-diffusion equation solver is utilized to obtain the electrical properties of the device. The carrier transport properties of organic material are quite different from the traditional semiconductor. While the electrons/holes transport though the organic materials, carrier will move to the other site by hopping in the molecular orbitals. The bandgap of organic material is the difference between the lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO). Fig.1(b) is the illustration of density of states that there are tail states in the organic materials, leading to two unique properties: (1) The absorption of the light in the range of wavelengths with photon energy smaller than the bandgap energy. (2) Carriers can transport around the bandgap by the hopping process.

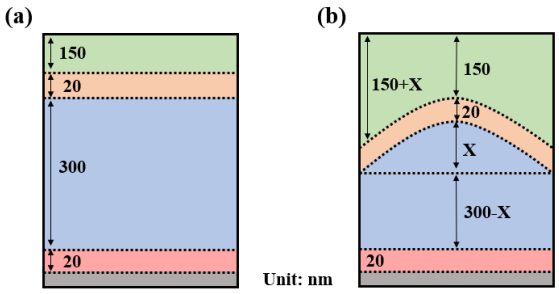


Fig. 2. (a) The structure of planar perovskite solar cells; (b) The structure of nano-structure perovskite solar cells, where X is the height of curvature.

## III. Result and Discussion

Fig.2(a) is our initial simulation structure of the planar perovskite solar cells. Fig. 4(a) is the current density-voltage(J-V) curve experimental fitting result of the $MAPbI_3$ solar cell. The experimental result was refer to this essay [1]. The characteristic parameters has shown in Table I. Under this fitted parameters, we want to know the optimization possibility of this structures. To improve efficiency of the solar cell, we should enhance the $J_{sc}$ first. Therefore, we would propose the designing a nano-structure to achieve this goal. [1] Since the diffusion length of $MAPBI_3$ is short [1], the thickness of $MAPbI_3$ was limited. We tested different thicknesses and found that 300nm thickness was the best for carrier extraction. Fig.2(b) is the nano-structure perovskite solar cells. Table. I show the characteristic parameters of nano-structure perovskite solar cells. Although the $J_{sc}$ increases merely a little bit due to the thickness limitation. However, the current flow path in $MAPBI_3$ is shorter. Fig.3 shows the generation map of different curvature. We can observe the light would be focus by nano-structure to enhance absorption. Furthermore, due to the effective length becomes shorter, this structure avoid the problem that the diffusion length of $MAPBI_3$ is so short that the efficiency become lower. Fig.4(b) show the fill factor is greater than planar's. And the 150nm height nano-structure have best efficiency than others. We considered the the ability of light-trapping would increase with longer curvature. Most importantly, the effective length would decrease with the increase of height.

TABLE I
THE CHARACTERISTIC PARAMETERS OF THE SIMULATION WITH PLANAR AND NANO-STRUCTURE.

| | $J_{sc}$(mA/cm$^2$) | $V_{oc}$ (V) | FF (%) | Efficiency(%) |
|---|---|---|---|---|
| Planar | 21.16 | 1.11 | 77.34 | 18.15 |
| X=50 | 21.05 | 1.12 | 77.42 | 18.24 |
| X=100 | 21.67 | 1.13 | 78.98 | 19.28 |
| X=150 | 21.45 | 1.14 | 80.68 | 19.67 |

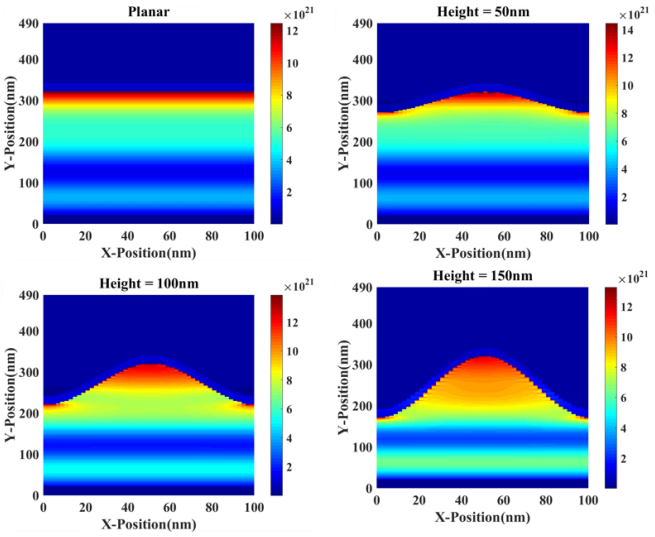


Fig. 3. The generation rate of the solar cells with different height of curvature.

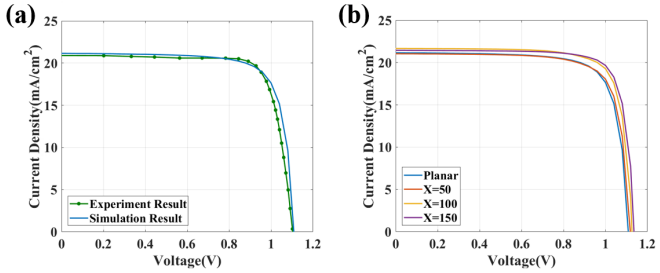


Fig. 4. (a) The J-V curves of the planar solar cells; (b) The J-V curves of the nano-structure solar cells.

## IV. Conclusion

To summarize, we've showed the fitting results about the 2D simulation of the planar $MAPbI_3$ solar cells. Further, we design a nano-structure that could increase the performance of $J_{sc}$ and $V_{oc}$ and this adjustment can have an increment of 1.5% in efficiency. Finally, the efficiency of $MAPbI_3$ based solar cell has been improved from 18% to 19.67%. Furthermore, we have established a 2D simulation tool that can analyse the performance of perovskite solar cells by optical properties and electrical properties. Hence, this tool can conduce to optimize perovskite solar cells.

## V. Acknowledgement

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## References

[1] J. H. Heo, H. J. Han, D. Kim, T. K. Ahn, and S. H. Im, "Hysteresis-less inverted ch 3 nh 3 pbi 3 planar perovskite hybrid solar cells with 18.1% power conversion efficiency," *Energy & Environmental Science* **8**(5), pp. 1602–1608, 2015.