

OPTICAL ABSORPTION STUDY OF PEROVSKITE SOLAR CELL WITH PHOTONIC CRYSTAL USING FDTD SIMULATION

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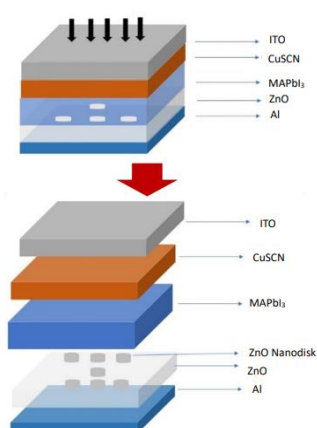
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Graphical abstract



Abstract

Increasing absorption poses a challenge for enhancing solar cell performance. Consequently, perovskite solar cells have emerged as a solution in recent years due to their advantages, such as high flexibility, low cost, and good radiation resistance. To further enhance the performance of perovskite solar cells, photonic crystals have been introduced into their structure, boasting exceptional optical properties. In this study, two-dimensional photonic crystals comprising ZnO material and MAPbI₃ perovskite were utilized as absorbent layers. Through Finite Difference Time Domain (FDTD) simulations, the research successfully demonstrates the effectiveness of increasing absorption by modifying the diameter and period of the photonic crystals. The results indicate that absorption increases as the diameter decreases and the period increases. Notably, the highest absorption value was achieved with a diameter of 0.20 μm and a period of 0.50 μm . The simulation results clearly illustrate that perovskite solar cells with photonic crystals exhibit higher absorption compared to solar cells without photonic crystals.

Keywords: Perovskite, solar cells, photonic crystal, optical absorption, FDTD simulations.

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1.0 INTRODUCTION

Perovskite solar cells have experienced rapid development in recent years and are classified as third-generation solar cells, offering numerous advantages over other types of solar cells. For instance, they possess high flexibility, allowing for design on flexible substrates [1], are cost-effective [2], exhibit a high absorption coefficient [3], and demonstrate superior radiation resistance compared to glass while providing very high specific power [1]. These exceptional attributes contribute to enhanced photoelectric conversion efficiency, positioning perovskite as a promising photovoltaic material for solar cells.

To enhance the performance of solar cells, such as absorption, photonic structures have been introduced in perovskite solar cells [4]. Photonic crystals are widely used in solar cells due to their unique optical properties, including the photonic bandgap and the "slow photon" effect. The photonic bandgap refers to the range of frequencies or wavelengths in which certain directions of photon propagation are prohibited within a photonic crystal. This bandgap is influenced by the periodic structure, affecting the speed of light passing through the crystal over the photon energy range [5].

When light propagates through a photonic crystal, the structure's periodic adjustment of the dielectric constant leads

to Bragg scattering, resulting in a band structure within the crystal. The scattering and wave interference effects provide the fundamental mechanisms for light trapping [6], [7]. The advantage of using photonic structures in solar cells is the ability to control absorption within the cells [8][9], manage light interaction as required [10], and significantly increase the External Quantum Efficiency (EQE) by an average of approximately 22% [11]. Achieving a higher external quantum efficiency requires optimizing the photonic crystal structures alongside achieving favorable photovoltaic characteristics, including charge mobility and recombination rates [12].

Photonic crystals are categorized based on their spatial period arrangements, including one-dimensional, two-dimensional, and three-dimensional structures, each exhibiting variations in materials and dielectric constants [3]. One-dimensional, two-dimensional, and three-dimensional photonic crystals offer several advantages, with higher-dimensional structures exhibiting superior optical properties. Among these, one-dimensional photonic crystals have been extensively studied and utilized due to their simplicity [13]. However, three-dimensional photonic crystals come with certain drawbacks, as their complexity necessitates advanced fabrication technologies [3].

Numerous studies have focused on employing two-dimensional photonic crystals in solar cell applications, including perovskite solar cells with nanodisk-shaped photonic crystals, which demonstrated an impressive absorption rate of 94% [4]. Additionally, solar cells with photonic crystals integrated into a silicon layer exhibited a substantial increase in the number of absorbed photons, resulting in an absorption rate of 56% [8]. In the case of organic solar cells, the utilization of photonic crystals led to enhanced absorption compared to conventional solar cells [14]. The benefits of photonic crystals are achieved when they are appropriately positioned [15].

In this study, 2D photonic crystals were employed by modifying the diameter and lattice constant to achieve optimal solar cell performance. The absorption was measured on the perovskite layer structure, designed using FDTD simulation. The objective of this research is to demonstrate that solar cells using photonic crystals outperform those without photonic crystals.

2.0 METHODOLOGY

In this study, Lumerical FDTD was utilized to analyze light absorption. The structure in the model consists of five layers with photonic crystals placed between the electron transport layer (ETL) and perovskite layer. The layer sequence, from bottom to top, comprises metal electrodes (aluminum - Al) with a thickness of 0.5 μm , ETL of zinc Oxide (ZnO) with a thickness of 0.7 μm , photonic crystals with a thickness of 1.2 μm , optimized diameter between 0.20–0.45 μm , and lattice constant ranging from 0.25–0.50 μm . Following that, the perovskite layer of MAPbI₃ has a thickness of 0.193 μm , hole transport layers (HTL) of Copper (I) thiocyanate (CuSCN) have a thickness of 0.05 μm , and transparent electrode layers of Indium-Tin-Oxide (ITO) with a thickness of 0.178 μm .

The geometric structure of each layer is defined in the XY, YZ, and ZX dimensions. Three monitors are strategically positioned to record the results, with two monitors placed at

the upper and lower limits of MAPbI₃. To observe the increase in absorption, the diameter and lattice constant of the photonic crystal structure were varied while maintaining a constant height. In the simulation, mesh points are used to calculate all inputs during the simulation, ensuring more accurate results by increasing the number of mesh points. Additionally, flat waves with a wavelength range of 300-900 nm are employed as electromagnetic sources instead of direct sunlight.

After conducting optical simulations, several important parameters were obtained. These parameters were obtained using a mathematical equation. The total power absorbed by the solar cell was evaluated by calculating the input absorbed by the solar cell at each wavelength. Mathematically, this process involves applying the divergence of the vector based on Equation (1):

$$P_{abs} = -0.5 \text{ real } \vec{\nabla} \cdot \vec{P} \quad (1)$$

The divergence calculation is utilized due to the shape being relatively stable, resulting in the modification of Equation (1) to become Equation (2):

$$P_{abs} = -0.5 \omega |E|^2 \text{imag}(\epsilon) \quad (2)$$

Where ω is the angular frequency, $|E|^2$ is the electric field intensity, and $\text{imag}(\epsilon)$ is the permittivity. The absorption can be calculated by the electric field intensity and the imaginary part of the permittivity can be calculated from the FDTD simulation [16]–[19].

3.0 RESULTS AND DISCUSSION

In this study, the solar cell structure used is ITO/CuSCN/MAPbI₃/ZnO/Al, as illustrated in Figure 1. CuSCN serves as a HTL, while ZnO functions as an ETL and acts as a photonic crystal material. The photonic crystals are positioned on the electron transport layer since it plays a vital role in carrying the generated electrons and suppressing charge recombination with holes, resulting in high charge mobility for the ETL [20]. To achieve optimal perovskite solar cell performance, parameters such as the diameter and lattice constant of the photonic crystals were varied. The photonic crystal diameter ranged between 0.20-0.45 μm , and the photonic crystal lattice constant varied between 0.25-0.50 μm .

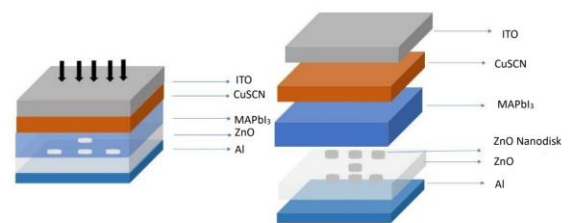


Figure 1 Structures of perovskite solar cells modified by photonic crystals

In addition to varying the diameter and lattice constant of the photonic crystal to increase absorption, material selection was also conducted to obtain the best PSC absorption value. MAPbI₃ material was chosen for this study due to its excellent absorption capability, with a maximum absorption reaching 92% [4]. Furthermore, using ZnO as the ETL and CuSCN as the

HTL contributes to optimal absorption, thereby enhancing the performance of the solar cells [21].

Figure 2a illustrates the effect of varying the diameter of the photonic crystal on absorption within the range of 300-900 nm. Notably, changes in diameter do not significantly affect the absorption in the 300-450 nm wavelength range, where the absorption remains relatively constant around 0.9. However, in the 450-900 nm range, absorption increases as the diameter of the photonic crystal decreases. Consequently, the optimal diameter observed in this simulation is 0.20 μm . In the wavelength range of 450-900 nm, a blue shift occurs as the diameter of the photonic crystal within the solar cell increases. This shift is caused by the photonic bandgap effect. The photonic bandgap effect occurs when the wavelength of light is proportional to the periodicity of the photonic crystal structure [22]. This bandgap causes the absorption of light to be suppressed in certain areas of the spectrum and enhances light absorption in other regions. In the 450-900 nm range, both transmission and absorption are improved, allowing the solar cell to capture various high-energy photons, thus increasing the overall efficiency of the solar cell [23].

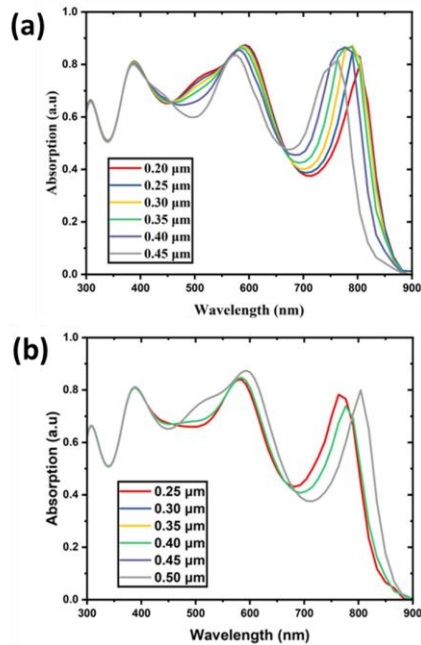


Figure 2 Structures of perovskite solar cells modified by photonic crystals

Moving to Figure 2b, it demonstrates the impact of changes in the photonic crystal lattice constant on absorption. In this case, variations in lattice constant, specifically 0.30, 0.35, and 0.40 μm , exhibit similar absorption values. Similarly, the 0.45 and 0.50 μm lattice constants also show equivalent absorption, indicating minimal differences between these values. Within the 300-450 nm wavelength range, the absorption remains constant at approximately 0.8. However, in the 450-900 nm wavelength range, the absorption value increases with the lattice constant's enlargement. Consequently, larger lattice constants lead to greater absorption values. This phenomenon is attributed to the periodic structure of photonic crystals, where light diffraction plays a crucial role in the formation of photonic bands and photonic band gaps (PBG). Larger lattice

constants facilitate light diffraction, resulting in an increase in absorption. Based on these observations, the optimal lattice constants obtained through this simulation are 0.45 and 0.50 μm . When increasing the photonic crystal lattice constant within the solar cell, it can affect the ability of this structure to absorb light [4]. A larger lattice constant can result in a redshift in the photonic crystal bandgap [24]. This means that the photonic crystal becomes more efficient in absorbing longer-wavelength light. The redshift of the energy gap caused by the larger lattice constant allows the solar cell to capture more photons with energy in the 450-900 nm range. Consequently, the solar cell can efficiently absorb light, leading to an overall improvement in the efficiency of the solar cell.

To ascertain the absorption enhancement attributed to the photonic crystal solar cells, the simulation was conducted with the optimal parameters for the photonic crystal, specifically a diameter of 0.20 μm and a lattice constant of 0.50 μm . As depicted in Figure 3, the absorption values within the wavelength range of 650-900 nm are notably higher compared to flat solar cells. This indicates that solar cells with photonic crystals exhibit superior performance over flat solar cells, primarily due to their enhanced optical absorption, particularly in the near-infrared region.

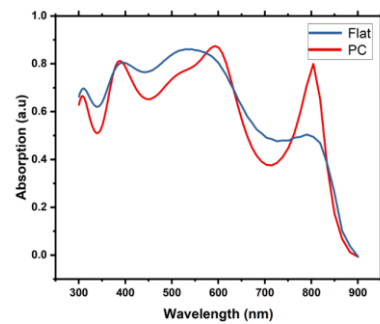


Figure 3 Absorption spectrum curves of solar cells with photonic crystals (PC) and flat solar cells

Figure 4 displays the distribution profiles of the electromagnetic field for perovskites with photonic crystals and perovskites without photonic crystals. In the figure, the red color signifies a high-intensity electromagnetic field, while the dark blue color indicates a low-intensity electromagnetic field. It is evident that the perovskite electromagnetic wave field with photonic crystals is more concentrated, whereas the perovskite electromagnetic wave field without photonic crystals appears more scattered and lacks a distinct center.

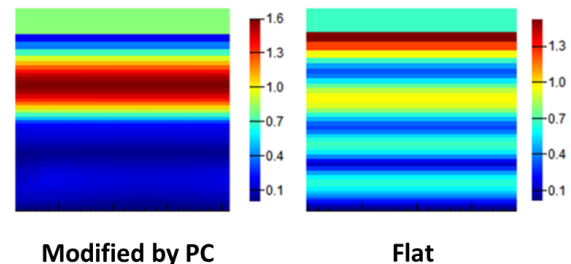


Figure 4 Electromagnetic field density profile of perovskite solar cells modified by photonic crystal (PC) and flat

4.0 CONCLUSION

In this study, we successfully improved the performance of photonic crystal-modified perovskite solar cells using FDTD (Finite-Difference Time-Domain) simulations. The photonic crystals were optimized by varying the diameter between 0.20–0.45 μm and the lattice constant between 0.25–0.50 μm . The results indicate that perovskite solar cells with photonic crystals exhibit the highest absorption values at a diameter of 0.20 μm and a lattice constant of 0.50 μm . The enhancement in absorption is observed with an increase in both the small diameter and the lattice constant. These findings demonstrate that the modification of perovskite solar cells using photonic crystals can significantly influence the solar cells' absorption performance. Furthermore, the performance can be finely tuned by adjusting the geometrical parameters such as the diameter and lattice constant of the photonic crystal.

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Conflicts of Interest

The author(s) declare(s) that there is no conflict of interest regarding the publication of this paper

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