

Key Factors Affecting the Efficiency of Perovskite Solar Cells

Haoze Xiong

*School of Materials Science and Engineering, Wuhan University of Technology, Wuhan, China
2788188261@qq.com*

Abstract. With the growth in global energy demand and increasing environmental protection requirements, perovskite solar cells have become a research hotspot due to their advantages of high efficiency, low cost, and flexibility. Its low-cost and easy-to-prepare characteristics can reduce the cost of photovoltaic power generation and expand the popularization of clean energy. High light absorption efficiency can increase the power generation per unit area and alleviate the constraints of land resources. After solving the stability issue, traditional silicon-based batteries can be supplemented or even partially replaced, enriching the clean energy system and accelerating the transformation of the energy structure towards low-carbon. This paper uses literature analysis and review methods to explore the factors affecting their efficiency and stability: the chemical composition (A, B, X ions) determines the photovoltaic performance, while humidity, temperature, oxygen, and light exposure can cause material decomposition, film quality degradation, and reduced efficiency. Research indicates that performance can be enhanced by adjusting material structure and optimizing operating conditions. In the future, once stability issues are resolved, their application prospects in the energy sector are vast, with the potential to drive the development of clean energy.

Keywords: perovskite, stability, efficiency, temperature, photo-oxidation

1. Introduction

As modern industry and urbanization continue to develop, energy demand is growing alongside worsening environmental pollution. Finding and utilizing sustainable green energy has become an important issue of concern. Solar energy, with its widespread availability, environmental friendliness, and endless supply, is widely utilized, particularly in solar cells.

In recent years, perovskite-based solar cells have seen rapid development. Perovskite solar cells are a type of solar cell that utilizes perovskite-type organic metal halides as light-absorbing materials. Perovskite solar cells have garnered significant attention due to their high efficiency, low cost, and flexibility. Therefore, perovskite solar cells have developed rapidly. A research team led by Dr. Yi Chenyi from the New Power System Research Center of the Carbon Neutrality Research Institute at Tsinghua University achieved the world's highest efficiency record of 26.41% for perovskite solar cells by developing new hole transport materials combined with vacuum-deposited perovskite thin films [1].

However, perovskite is highly sensitive to environmental conditions, with factors such as temperature, humidity, and light exposure leading to perovskite decomposition and reduced cell efficiency. Therefore, further improvements in the stability of perovskite solar cells are necessary. Additionally, due to differences in the composition and structure of perovskite itself, both the operational efficiency and lifespan of the cells are affected to varying degrees. This paper employs literature analysis and review methods to summarize and discuss some of the factors influencing the efficiency of perovskite solar cells. The objective of this paper is to discuss the factors affecting the stability of perovskite solar cells and explore reasonable methods to enhance their efficiency.

2. Perovskite and perovskite solar cells

2.1. Perovskite

Perovskite refers to a class of inorganic-organic hybrid materials with the molecular formula ABX_3 , where A is typically a monovalent cation such as methylammonium or cesium, B is a divalent metal cation such as lead or selenium, and X is a halide anion such as chlorine, bromine, or iodine. The crystal structure of perovskite is highly flexible, ideally cubic symmetrical, with A-site ions occupying the octahedral voids formed by B-site and X-site ions. This structure facilitates the separation and transport of electrons and holes, thereby enhancing photoconversion efficiency. Additionally, the bandgap width of perovskite materials can be adjusted by modifying their chemical composition. Therefore, perovskite materials are materials with excellent optical properties.

2.2. Perovskite solar cells

Perovskite solar cells (PSCs) are solar cells that utilize perovskite-type organic metal halides as light-absorbing materials. Their basic structure typically includes a transparent conductive oxide layer (TCO) such as fluorine-doped tin oxide (FTO) or indium-doped tin oxide (ITO) as the glass substrate, followed by an electron transport layer (ETL), perovskite, a hole transport layer (HTL), and metal electrodes. When sunlight strikes the perovskite layer, photons are absorbed and excite electron-hole pairs. The electrons and holes rapidly separate and are transported to the electron transport layer and hole transport layer, respectively, thereby generating a current and converting light energy into electrical energy.

3. Key factors affecting the efficiency of perovskite solar cells

3.1. Chemical composition

Perovskite has an ABX_3 structure, containing monovalent cations (A^+), divalent metal cations (B^{2+}), and halide ions (X^-). Altering these chemical components can modify the physical and chemical properties of perovskite, thereby affecting the efficiency and lifespan of perovskite solar cells.

3.2. Organic cations

Taking the common perovskite cell $CH_3NH_3PbI_3$ as an example, its bandgap width is 1.68 eV. Altering the size of the cations can change the bond length and bond angle of Pb-I, leading to changes in the crystal structure and thus the bandgap. For instance, replacing methylamine with larger cations reduces the bandgap, causing the absorption edge to shift toward the red end of the

spectrum and significantly enhancing near-infrared light capture capability. Improving carrier efficiency [2].

3.2.1. Halide anions

The types and proportions of halide anions can influence the bandgap structure of perovskite materials, thereby affecting their absorption range and efficiency for sunlight. For example, in mixed halide perovskites, adjusting the ratio of iodine ions to bromine ions can achieve tunable bandgap structures, enhancing the photoconversion efficiency of solar cells. Herz et al. found in their experiments that the carrier mobility of $\text{MAPbI}_{3-x}\text{Cl}_x$ and MAPbI_3 was 11.6 and 8 $\text{cm}^2/(\text{V}\cdot\text{s})$, respectively, indicating that mixed halide perovskites have higher mobility, resulting in higher efficiency in solar cells [3].

3.2.2. Metal cations

The type and properties of metal cations directly influence the bandgap, light absorption coefficient, carrier mobility, and other photovoltaic performance parameters of perovskite materials. For example, lead-based perovskites have become the mainstream material for perovskite solar cells due to their excellent photovoltaic properties. However, due to lead toxicity concerns, lead-free perovskite materials such as tin and germanium have also been developed. The performance of these lead-free perovskite materials largely depends on the choice of metal cations. Lead-tin mixed perovskites extend the wavelength absorption of the original $\text{CH}_3\text{NH}_3\text{PbI}_3$ from 800 nm to 1060 nm, while tin halide perovskites achieve up to 1250 nm. By doping or replacing metal cations, the bandgap structure of perovskite materials can also be adjusted to optimize their absorption range of sunlight, thereby enhancing photovoltaic conversion efficiency [4].

3.3. Humidity

Humidity is one of the key factors affecting the performance and stability of perovskite solar cells. During the preparation and use of perovskite solar cells, it is essential to comprehensively consider the impact of humidity on both cell preparation and stability. Therefore, understanding the effects of air humidity on cells is of significant importance for industrial-scale production. The two-step spin-coating method is widely used due to its ability to control the size of perovskite particles. In experiments conducted by Jiang Jiajia et al., the impact of environmental humidity during the preparation process on the performance of perovskite solar cells was investigated [5]. When PbI_2 solution is spin-coated on an FTO/dense TiO_2 /porous TiO_2 substrate, the formation of the PbI_2 film is influenced by moisture.

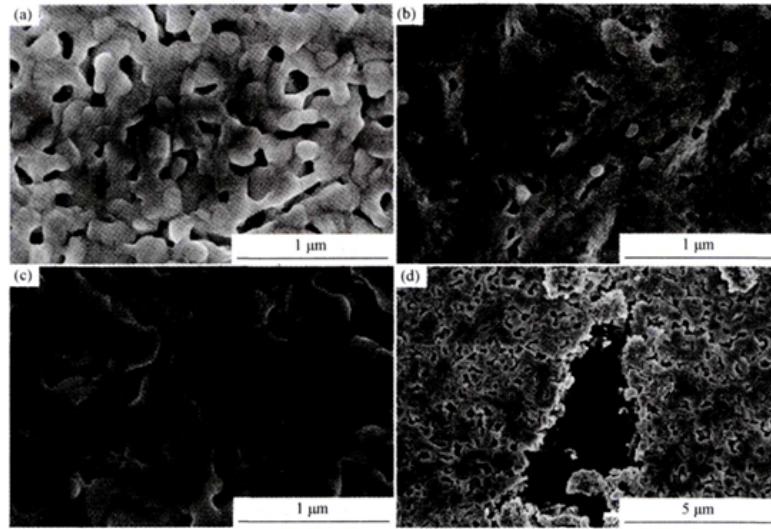


Figure 1. FE-SEM images of the PbI₂ thin film surface at different humidity levels: (a) 15%; (b) 40%; (c) 70%; (d) 70%

In the FE-SEM images of the PbI₂ film surface and the perovskite film surface (see Figure 1), at 15% humidity, the PbI₂ film surface exhibits some pores, while the perovskite film remains dense and intact. At 40% humidity, the PbI₂ film surface is smooth and dense, while the perovskite film exhibits pores. When humidity reaches 70%, the PbI₂ film develops numerous pores, and the incomplete nature of the PbI₂ film significantly reduces the coverage of the perovskite film. Additionally, the perovskite particles gradually transform from their original cubic shape into irregular shapes. The coverage of the perovskite film decreases with increasing humidity, which reduces the battery's light absorption capacity, decreases the number of excited carriers, and lowers the short-circuit current density. Additionally, low coverage causes the hole transport material (HTM) to come into direct contact with TiO₂, leading to carrier recombination and HTM decomposition, which affects the short-circuit current density and open-circuit voltage, ultimately impacting battery efficiency. In the experiment, the cell efficiency decreased from 8.96% to 7.05%, and at 70% humidity, it dropped to 3.61%.

3.4. Temperature

The thermal stability of perovskite solar cells is one of the key factors affecting their long-term development and commercial application. At higher temperatures, perovskite materials may decompose and undergo phase transitions, affecting the cell's open-circuit voltage (VOC) and short-circuit current density (JSC). In Qimeng's experiment, significant changes in perovskite films were observed under varying temperatures [6]. As the processing temperature increased and the processing time prolonged, the originally black films turned yellow, and the photoconversion efficiency of perovskite solar cells decreased linearly. Further investigation into the effect of temperature on perovskite thin films. Figure 2 shows the XRD spectra of perovskite thin films processed for 70 minutes at different temperatures (25°C, 8°C, 100°C, 150°C, 200°C, and 250°C).

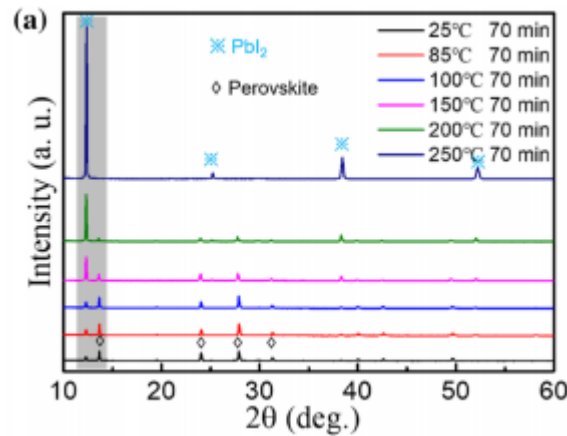


Figure 2. XRD patterns of perovskite films treated for 70 min at different temperatures (25°C, 8°C, 100°C, 150°C, 200°C, and 250°C)

Observing the perovskite peaks, it was found that varying amounts of lead iodide appeared on the treated films. The experiment demonstrated that perovskite decomposes into PbI_2 at high temperatures. As shown in SEM Figure 3, the higher the temperature, the more PbI_2 accumulates on the surface of the perovskite film. The generated PbI_2 hinders the movement of charge carriers in the battery, causing electron-hole recombination, which results in a linear decrease in the battery's VOC and thus affects battery efficiency.

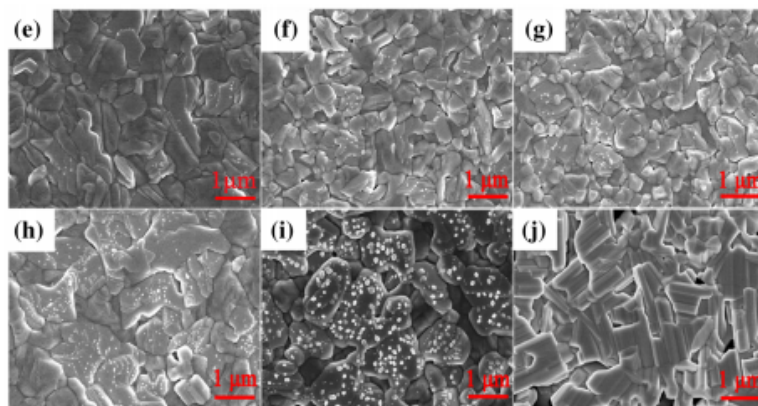


Figure 3. SEM images of perovskite thin films heated for 70 min at different temperatures: (E) 25°C; (f) 85°C; (g) 100°C; (h) 150°C; (i) 200°C; (j) 250°C

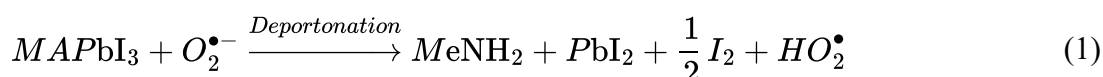
For short-circuit current density (JSC), there is a linear relationship between JSC and temperature in traditional solar cells. However, in perovskite solar cells, this relationship is not entirely linear [7]. As the bandgap increases, the ideal current decreases, while the collection efficiency increases with rising temperature. Different factors dominate different situations, and JSC may either increase or decrease. This affects the efficiency of perovskite solar cells.

3.5. Oxygen and light exposure

Oxygen and light-induced degradation are also important factors affecting the performance and stability of perovskite solar cells. When manufacturing low-cost, high-efficiency perovskite solar cells, oxygen and light-induced degradation are factors that must be considered. Oxygen-induced

degradation is a method of regulating the electrical properties of organic and inorganic electron transport layers. Under dark conditions, the oxygen-induced degradation reaction in perovskite solar cells is generally weak. WANG et al. pointed out that under dark conditions, oxygen acts solely as a p-type dopant and does not react with MAPbBr₃ [8]. However, when perovskite materials are simultaneously exposed to oxygen and light, the films exposed to light and oxygen undergo severe degradation, resulting in a significant decrease in film absorbance.

This is because light-accelerated degradation under oxygen conditions may form superoxide ions O₂^{•−}, which possess strong nucleophilic properties. These superoxide ions can react with the organic cations in the perovskite through a deprotonation process as follows:



The volatilization of its products causes irreversible decomposition of perovskite, leading to a decline in the performance of perovskite solar cells.

4. Conclusion

This paper primarily discusses the factors affecting the stability of perovskite solar cells and explores reasonable methods to enhance their efficiency. Perovskite solar cells have demonstrated exceptional performance and cost-effectiveness in the energy sector, making them highly competitive in the battery field. The high light absorption and mobility characteristics of perovskite crystals enable the cells to achieve high efficiency. However, the most pressing issue currently facing perovskite cells is their stability. Identifying suitable perovskite crystals, preventing water from damaging the crystal structure of perovskite, mitigating the impact of high temperatures on the uniformity of the perovskite light-absorbing layer, and reducing the effects of photo-oxidation on perovskite crystals are essential to maintaining the stability and efficiency of perovskite solar cells.

In summary, by adjusting the structure of perovskite solar cells, modifying the properties of internal materials, and upgrading operating conditions, the efficiency of perovskite solar cells will achieve significant breakthroughs.

References

- [1] Wolfgang Tress, Simone Meloni, Chenyi Yi. Highly efficient and stable perovskite solar cells via a multifunctional hole transporting material [J]. Joule, 2024: 1691-1706.
- [2] Borriello I, Cante G, Ninno D. Ab initio investigation of hybrid organic-inorganic perovskites based on tin halides [J]. Phys. Rev. B, 2008: 77(23), 235214
- [3] Wehrenfennig C, Eperon GE, Johnston MB, Snaith HJ, Herz LM. High charge carrier mobilities and lifetimes in organolead trihalide perovskites. [J] Adv Mater, 2014; Mar 12; 26(10)
- [4] Ogomi Y, Morita A, Tsukamoto S, et al. CH₃NH₃Sn_xPb_(1-x)I₃ Perovskite Solar Cells Covering up to 1060 nm. [J]. Journal of Physical Chemistry Letters, 2014, 5(6): 1004-1011.
- [5] Jiang Jiajia, Cao Fangxu, Wang Kang, Tan Bin, Tao Haijun. Effect of humidity on the performance and stability of perovskite solar cells [J]. Journal of Materials Science and Engineering, 2017, 35(2): 181-186.
- [6] Meng Q, Chen Y, Xiao Y Y, et al. Effect of temperature on the performance of perovskite solar cells [J]. Journal of Materials Science: Materials in Electronics, 2020(6156).
- [7] Schwenzer J A, Rakocevic L, Gehlhaar R, et al. Temperature Variation-Induced Performance Decline of Perovskite Solar Cells. [J]. ACS Applied Materials & Interfaces, 2018: acsami.8b01033.

- [8] Xin-Xin P, Danyal A, Fei L, et al. Oxygen-and photo-induced decay of perovskite solar cells: Mechanisms and strategies [J]. Journal of Central South University, 2024, 31(12): 4366-4396.