Perovskite Solar Cells: Structure, Working Principle, and Modification Strategy

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Abstract. Perovskite solar cells (PSCs) are known for their excellent photoelectric conversion efficiency, low cost, and high flexibility. Organic-inorganic hybrid PSCs have excellent performance which is comparable to traditional solar cells. However, the crystal quality of perovskite thin films is poor. In addition, there are numerous interface defects in the films, which lead to the unstable performance. Therefore, exploring ways to modify PSCs is beneficial for expanding their application realms. This work mainly discusses the development of perovskite solar cell. The structures of PSCs are discussed. The components and working principles of PSCs are described in detail. Perovskite films exhibit many defects, especially at the interface. These defects hinder the movement of charge carriers. As a result, the lifetime of charge carriers is largely reduced. Defect passivation technology can help improve this situation. Therefore, this work also introduces the modification strategies of PSCs including the additive engineering and interface engineering. In addition, exploring two-dimensional perovskite materials as one of the effective ways of modification has also been summarized. This work opened up a new perspective for the study of PSCs.

Keywords: Perovskite solar cell, Modification, Structure, Passivation.

1. Introduction

With the raising awareness of the pollution issues, exploring new energy becomes the best choice for people. Nowadays, the problem of energy shortage is stressed and the environment-friendly way of energy use is encouraged by the government. Especially in the northwest of China, because of the high altitude and low land utilization rate, solar energy is considered to be an important energy in this region. Solar energy becomes the important part for the energy revolution. Exploring ways to achieve high energy-conversion efficiency is the pursuit of researchers in this field.

Considering these factors, perovskite solar cells (PSCs) have become a research hotspot [1-3]. The incident photon-to-electron conversion efficiency (IPCE) is regarded as a key indicator for PSCs. PSCs exhibit high IPCE which is up to 25%. Meanwhile, the theoretically IPCE rate of PSCs is very high, which means that PSCs have great research value. Furthermore, PSCs also have low cost and adjustable components. There are various types of perovskite materials, which have the advantages of diverse structures and adjustable properties. Perovskite materials include traditional inorganic perovskites, organic-inorganic hybrid perovskites, and pure organic perovskite materials. The introduction of organic components makes perovskite materials flexible. This feature has opened up new application areas of flexible devices for PSCs. PSCs have potential applications in automobiles, domestic electricity consumption or even satellite. Although there are a lot of advantages for PSCs, there are still some limitations in this technology. PSCs have lower durability when they are compared to the traditional silicon solar cells. Lead poisoning during the processing or using is also a restriction of PSCs. Therefore, PSCs have been extensively studied in recent years [4-6].

This work mainly discusses the PSCs. The researches on PSCs in recent years are outlined. The modification methods for this technology are also discussed in detail.

2. Structure and Working Principle

When photons reach the surface of PSCs, energy transfer is completed by forming excited electrons. Electron-hole pairs are generated as a result. These electrons are negative and they can move freely. Meanwhile, the holes they leave behind are positive carriers. Due to the built-in electric field within the solar cell, the separated electrons and holes are pushed in opposite directions. This creates a flow of electric current.

PSCs utilize materials with perovskite structure as the active layer [3]. Perovskite materials have a crystal structure of ABX_3. Based on this material, PSCs are constructed.

The light-absorbing layer of PSCs is perovskite materials [6-8]. These materials can be organometallic halides, such as methylammonium lead iodide ($CH_3NH_3PbI_3$). When sunlight strikes the perovskite layer, the electrons are excited, creating electron-hole pairs similar to traditional silicon-based solar cells. The electron-hole pairs separate in the perovskite layer due to the unique electronic structures. The electrons move to one side of the cell, while the holes move to the other side. This separation creates an electric field, facilitating the flow of electrons, which can be harvested as electrical current. PSCs display high efficiency in converting sunlight into electricity. The efficiency record for PSCs has been rapidly increasing. It has already exceeded 25% in laboratory settings which is comparable to the efficiency of traditional silicon solar cells.

Currently, PSCs that have planar construction are commonly used. PSCs can be divided to two types, including regular planar structure (p-i-n) and inverted planar structure (n-i-p). In p-i-n structure, PSCs are composed by metal electrode, hole transport layer (HTL), perovskite, electron transport layer (ETL) and the transparent substrate. However, in most circumstance, there are some layers insert into the PSCs to achieve the passivation.

The most important part in the PSCs is the perovskite material. It can quickly complete the generation of electrons, accompanied by the formation of charged carriers. The chemical structure of typical perovskite is ABX_3. The cation A refers to methylamine or formamidine. For the B cation, Pb or Sn is often used. As to the X anion, people always use I or Cl. Till now, a large amount of works are conducted on PSCs, which have improved their IPCE. Exploring ways to solve the durability problem of PSCs is still worth studying. The reason why many PSCs are not put into production is that they cannot be maintained in the natural environment. Improving the stability of perovskite materials is the important research direction nowadays.

ETL is composed of a semiconductor material with high electron affinity and ionic potential energy. Its role is to help the electron hole pair separate. At present, the mainstream research direction is to optimize the structure and surface of ETL. Besides, improving the electron mobility and reducing the generation of UV-induced defects are also important research topics.

The function of HTL is to take over positively charged holes. HTL is mainly divided into three categories, including inorganic, polymer, and self-assemble monolayers (SAM). The first category is inorganic. In this category, nickel oxide is the best example. But the problem is that the efficiency is relatively low. As to the polymer type, the stability of this material is high. But the disadvantage of this material is poor infiltration, resulting in ion migration. It is difficult to form a film for this material. SAMs are single-layer films prepared by using self-assembly technology. Optimizing the structure and composition of SAMs attracted much attention of researchers.

According to previous reports, improving SAMs can enhance the solar power generation efficiency and reduce losses of PSCs. A trans-parallel perovskite structure can be used to achieve this modification. It is well acknowledged that HTL is lack of infiltration, resulting in the defect of ion migration. Therefore, molecules are added to the SAM layer to improve the side effects. Three molecules are screened, which have carboxylic acids and benzene rings in their structures. The structure of the solar panel from top to bottom include perovskite, SAM layer, and nickel oxide. It is found that the molecules in the original structure are prone to the appearance of trimers and tetramers. This leads to the formation of holes in nickel oxide and the migration of ions. Through numerous attempts, the polymerization phenomenon is reduced, which greatly reduces the appearance of holes.

There is also an important concept about energy level matching in PSCs. When solar energy is absorbed, the electrons will transition from the valence band to the conduction band, forming electron hole pairs. The energy provided by photons needs to enable excited electrons to cross the energy gap.

In fact, the band structure in perovskite is influenced by various factors, including chemical composition and defects.

3. Modification

Through continuous exploration, the structure of PSCs devices has become relatively stable. Optimizing the device structure is not able to achieve performance enhancement significantly, so new modification strategies still need to be explored.

Passivation is one of the main methods for modifying PSCs [4, 5]. The most common situation is that the metal reacts in chromic acid or chromate solution to form a film. The metal will not be oxidized in the natural environment and will remain more durable as a result of the film. In PSCs, because the perovskite itself is prepared by solution, there are many defects on its surface. By passivation, it can improve the power generation efficiency of perovskite solar energy and improve its durability. The perovskite can be passivated by several ways.

3.1. Interface Engineering

There are a large number of defects on perovskite thin films, which have a pinning effect on charge carriers. Meanwhile, these defects also can also decrease the lifetime of charge carriers. It is a serious obstacle to the improvement of V_{OC} in PSCs. According to reports, the ETL/perovskite interface also contains a large number of defects, which is an important factor limiting the efficiency of the cells. Meanwhile, the energy-level matching between ETL/perovskite interfaces is crucial for improving carrier extraction efficiency.

Grain boundary (GB) is an important part of the study to improve the degree of passivation. In many cases, the defect of grain boundary will lead to serious non-radiative recombination in perovskite. The GB refers to the boundary between grains. As for the boundary inside the grains, especially some large grains, there are often many large cracks, which can also lead to holes.

Some materials, including TiO_2 and SnO_2, have been introduced to improve this high-density defect structure [5]. In addition, the introduction of an intermediate layer composed of polymers can also achieve passivation [6].

3.2. Additive Engineering

Additive engineering is a control strategy for passivating defects in the perovskite absorber layer [8]. The role of additives is mainly auxiliary, and its role is mainly to stabilize the form and passivate some defects. The current mainstream of additives are ionic liquids (ILs), fullerene derivatives, and polymer polymers.

ILs have a wide thermal working range, which can reach -90^{o}C to 300^{o}C in some cases. Perovskite precursor solutions usually need to be treated over a wide temperature range. Therefore, ILs exhibit good performances in PSCs additive engineering. The research results indicate that the $MAPbI_3$ film treated with ILs has a smooth morphology and uniform coverage.

The indigo molecules are proposed to prepare perovskite films. Through explorations, it is proved that the passivation phenomenon can be achieved and the mobility of ions can be reduced. This method increased the optimal power conversion efficiency (PCE) from 20.18% to 23.22%.

3.3. Two-Dimensional Perovskite

The stability of PSCs largely depends on the morphology of the perovskite absorber [7]. Perovskites can be divided into layered and non-layered, which are composed of different structures. Layered perovskite structures typically include Ruddlesden-Popper (RP) and Dion-Jacobson (DJ). The layered structure has better adaptability than the non-layered ones. The single layer of perovskite in the layered perovskite is also called two-dimensional (2D) perovskite. Because it is extremely susceptible to external stimuli, such as pressure, bending and so on. Now there are many aspects of two-dimensional perovskite that need to be considered, such as the formation process of layered films.

In one article, methylamine lead iodine perovskite is prepared by hot steaming. A passivation layer is deposited on the surface by vapor deposition. The entire configuration is an RP perovskite. According to this paper, when there is more methylamine lead iodide in the structure, the carrier transport rate will be correspondingly improved.

4. Conclusion

PSCs are members of solar cells with excellent performance and research potential. This article discusses the structure and properties of PSCs. The working mechanism and common device structure are also discussed. Besides, the modification strategies for improving the performance of PSCs devices are also outlined. Overall, PSCs hold great promise for the future of solar energy technology. Continued researches which aim to further improve their efficiency, stability, and scalability are still needed. In the future, enhancing the stability of perovskite materials would contribute to broaden the application of PSCs. Meanwhile, exploring new lead-free perovskite materials will greatly promote the development of PSCs.

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