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Recent Advances in Carbon Nanotube Research for Perovskite Solar Cells

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Abstract. Although the photoconversion efficiency of perovskite solar cells (PSCs) has increased at a burgeoning rate, it has not been able to be commercialized due to the stability of the device and environmental hazards. Carbon nanotubes (CNTs) are highly conductive, flexible, and chemically stable; a systematic review of their multifunctional application in PSCs is presented in this paper: as an interface layer to maximize charge extraction and minimize recombination; as an active layer additive to control crystallization and passivate defects; as an encapsulation component to promote stability. Studies show that CNTs can be used to improve the overall performance of devices in several aspects and it is a good solution to simultaneously overcome the efficiency, stability, and environmental issues of PSCs. Among the most important areas of concern in the future, one should consider material system, fabrication process, design of a device structure and mechanistic research, and commercialization pathways.

Keywords: Carbon nanotubes, Perovskite solar cells, Interfacial layers, Crystallization regulation, Device stability

1. Introduction

Solar photovoltaic (PV) technology offers a key pathway to mitigating climate change by significantly reducing greenhouse gas emissions [1]. As a third-generation photovoltaic material, PSCs have rapidly become a hot topic of research in this field because of their excellent optoelectronic properties, including high carrier mobility, high defect tolerance, and high light absorption coefficients. In just over a decade, the photoconversion efficiency (PCE) of PSCs has risen from 2.2% to over 26% [2], demonstrating tremendous potential for practical applications.

However, despite such rapid progress, the commercial application of perovskite solar cells still faces several key obstacles: (1) Perovskite thin films contain a significant number of defects in both the bulk and on the surface, which severely affect their stability; (2) The device lacks long-term operational stability under environmental stresses such as moisture, heat, and light; (3) Environmental risks associated with lead leakage from damaged components.

Due to their hydrophobicity, flexibility, chemical stability, and extremely high carrier mobility and electrical conductivity [3], carbon nanotubes are considered an ideal material for enhancing the performance of PSCs. This paper aims to provide an overview of the multifunctional applications of CNTs in PSCs. The paper first analyzes the role of CNTs as an interface layer; second, it reviews

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their function as additives in modulating the perovskite layer; third, it summarizes their contributions to encapsulation and stability; and finally, it discusses current challenges and offers a look ahead, with the aim of providing guidance for advancing the commercialization of carbon nanotube-based perovskite solar cell technology.

From my perspective, CNTs have many undiscovered functions yet to be explored. The metallic or semiconducting properties exhibited by CNTs are worth further investigation and practical application.

2. CNTs as an interfacial modification layer

2.1. The role of the interface layer and the advantages of CNTs

PSCs operate based on the photovoltaic effect, where light irradiation on light-absorbing materials generates photo-generated electrons and holes. The detailed mechanism is as follows: (1) Light absorption and electron-hole pairs generation: When sunlight hits the light-active substance of PSCs, the perovskite material absorbs photons and produces electrons and holes. During the light absorption, these electrons and holes are excited and separated. (2) Carrier transport and separation: The electrons and holes generated are immediately separated in the perovskite layer and transported to the front and back electrode respectively. (3) Charge collection and current output: The electron transport layer (ETL) and the hole transport layer (HTL) are effective in transporting electrons and holes to corresponding electrodes. (4) Production of electric current: Via the external load circuit, when electrons and holes are brought in and out of the battery, a closed circuit is produced thus producing an electric current. Light energy is thus transformed into electrical energy and this is finally fed to the outer circuit or stored.

According to the foregoing operating principles, interface layers at every interface in the battery structure are very important in interface stability and carrier extraction. The integration of CNTs has several applications such as inhibition of carrier recombination and halide ion diffusion, optimization of alignment of energy levels, increased hole extraction, and passivation of defects, thus, enhancing the efficiency of PSCs.

The interface layer of carbon nanotube improves the performance of the device in three main ways. First, the functionalization of the surface by incorporating groups, e.g. carboxyl or -NH_2, can be done to tune the work function to favor the closer matching of the energy states of each layer and, consequently, to lower the energy barrier to carrier extraction. Second, fast pathways of charge transport can be formed by carbon nanotube networks, and this can greatly decrease carrier accumulation and recombination at interfaces. Third, a high concentration of CNTs can be used as a physical barrier, which restricts the movement of ions in the perovskite and the diffusion of atoms in the metal electrodes, which increases the life of the device.

2.2. Improving charge extraction efficiency

In apparatus with carbon as counter electrode, the lack of an efficient electronic barrier at the perovskite/carbon interface makes photo-generated electrons and holes recombine readily at the interface resulting in serious carrier recombination and a sharp reduction in the open-circuit voltage (Voc). Moreover, defects in the interface may serve as centers of charge recombination, further deteriorating the work of devices.

To overcome such concerns, the use of CNTs can establish an expedited carrier transport route, which will tremendously increase the efficiency of charge extraction and the performance of the

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device. Experimental research has indicated that the incorporation of self-passivated carbon nanotubes having coal-tar derived carbon structure at the perovskite HTL interface can be used to increase the photoconversion efficiency of 11.99 to 14.25 percent by promoting the induced effects produced by their oxygen-containing surface groups [4]. These findings will support the strong importance of carbon nanotubes to improve the hole conductivity of carbon electrodes and decrease the interfacial recombination resistance at the perovskite/carbon interface.

2.3. Passivation defects and inhibition of ion migration

These crystal defects that occur in perovskite crystals have a severe effect on carrier transportation and greatly affect photoconversion efficiency and long-term stability.

About interfacial defects, it has been discovered by the researchers that adding carbon nanotubes to the work function of the carbon electrode and to optimize the energy band structure of the nanotube can successfully reduce interfacial defects and maximize the efficiency in charge transport. Better energy-level matching is more efficient in collecting holes and it increases stability of the device.

Moreover, by integrating -NH_2 functionalized nanotubes of carbon on the perovskite grain boundaries, the defects are passivated by strong coordination of the amino functional groups with the uncoordinated Pb^{2+} ion. Meanwhile, the network of carbon nanotubes provides connectivity to the neighboring grains, which improves charge transport, and eventually a device efficiency of 21.01% is obtained [5]. On the whole, the interface layers of the CNTs are multifunctional, such as optimization of the energy levels alignment, charge transport, and stability of devices, which is an efficient method of improving the activity of PSCs.

3. CNTs as additives in perovskite layers

Carbon nanotubes that are functionalized and incorporated in perovskite layers have developed beyond basic conductive additives to multifunctional crystal growth regulators. The incorporation of trace levels of CNTs, through the use of CNTs as nucleation templates, through growth kinetics, and passivation of grain boundaries, allows the creation of high-quality perovskite films with larger grains and fewer defects. This is among the major processes in the production of high efficiency solar cells.

3.1. Evolution of features

The early studies concentrated more on the action of CNTs in the creation of charge bridges between grains and the purpose of increasing carrier transport. Nevertheless, later experiments indicated that perovskite films containing CNTs contained much larger grains with fewer defects implying that carbon nanotubes could have taken part in the crystallization process. Since the evolution of research, it has been evident that the doping of perovskite layers with low concentrations of functionalized carbon nanotubes can inherently enhance the quality of the film, and its advantages are not limited to the improvement of electrical conductivity. The role of the CNTs has therefore changed to that of a bridge to a pathway in charge transport to that of a template to control crystal growth.

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3.2. Mechanism of action

The mechanisms behind it are many processes that are coordinated. To prevent formation of defects, functional groups on the surface of CNTs (like -NH_2 and -COOH) react with lead ions (Pb^{2+}) in the perovskite precursors, which provide preferential nucleation sites, leading to growth of crystals along the surface of CNTs. Second, CNTs network structure is capable of modifying the kinetics of crystallization, which usually decreases the rate of crystallization by a moderate factor, giving the grains additional time to develop, leading to larger, intact grains. Once the crystallization is over, the CNTs do not leave the grain boundaries, with their functional groups still binding to defects by uncoordinated Pb^{2+} ions [5]. In the end, all these mechanisms will result in more quality and defect-free perovskite films.

3.3. Typical application strategies

A number of sufficient mechanisms have been devised to use functionalized CNTs as additives in the perovskite layers. As an illustration, Lin et al. used carboxylated carbon nanotubes (COOH-CNTs) in the perovskite precursor. Introduction of COOH-CNTs facilitates crystallization, grain size, decrease of defects and light absorption. In the case of devices using the $(FAPbI_3)_{0.97}(MAPbBr_3)_{0.03}$ system, the efficiency was improved to 18.91% with the addition of COOH-CNTs [6].

Also, a single study employed 4,6-di(anthracen-9-yl)-1,3-phenylene bis(dimethylcarbamate) (DPB) modified single-walled CNTs as crystallization templates. The carbamate moiety of the DPB molecule is a Lewis base which reacts with Pb^{2+} to form an effective Lewis acid-base complex, thereby passivating the defect; Simultaneously, the polyaromatic end groups of the CNTs stabilize the dispersion of the CNTs. DPB-functionalized CNTs are found to be more dispersive in perovskite precursor solvents and thereby allow uniform doping. Perovskite thin films synthesized in this way have a grain size larger than 500 nm and the device efficiency is also 20.7 percent, much higher than the 18.4 percent of the reference device [7]. This piece of work shows that this strategy does not only help to enhance the quality of the film but also it goes a long way to make device to work better.

Lewis base polymer-CNT composites are another strategy that is to be used as co-additives. The trap states are passivated by this polymer, which forms Lewis adducts with under-coordinated Pb^{2+} ions, and charge transport is accomplished by highly conductive carbon nanotubes, overcoming the conductivity limitations of the polymer itself. This plan eventually reached an efficiency of 21.7 percent in small devices and 20.7 percent in large devices [8].

4. The role of CNTs in encapsulation and stability enhancement

4.1. As a waterproof encapsulation barrier

The conventional packaging materials are restricted by flexibility, density, or price. Conversely, it is important to extend the implementation of CNTs to the outside of the device to the outside encapsulation in order to avoid the deterioration of the performance of PSCs in the long-term. Its mechanism of action is founded on two main factors: first, hydrophobicity of CNTs and, second, the high density of the network that the intertwining forms creates a considerable physical barrier that does not allow the water molecules and the oxygen to enter the CNTs; second, CNTs are very chemically stable, which means that they will not be degraded in harsh conditions and, therefore,

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will be able to protect the environment. Research has indicated that when carbon nanotube films are encapsulated, the resistance of the device to humidity and heat may enhance greatly. Indicatively, one study reported the use of a nano-hybrid film made of hydrophobic CNTs together with polymer hole-transport materials as a charge collector, allowing all-inorganic perovskite solar cells to continue operating with an efficiency of more than 4,000 hours in air without encasing the material, which is a remarkable stability indicator [9]. This shows its ability to design effective and dependable packaging systems.

4.2. As a lead leakage inhibitor and adsorbent

The dense structure of CNTs networks can be used effectively as a barrier to moisture and ions, in addition to the above-discussed physical protective properties, which are useful in tackling the severe environmental problem of lead leakage. Encapsulation technology of carbon nanotube is effective in enclosing the toxic lead ions within the device through exclusion of moisture hence reducing the chances of contamination of soil or water in the event of accidental damage of the device.

It should be mentioned that the roles of CNTs are not only restricted to encapsulation layers. Wang and colleagues came up with polyacrylic acid-grafted carbon nanotubes (CNT-PAA) in their work as an additive to the perovskite precursor. Specifically, the carboxyl-rich PAA units are able to interact with Pb^{2+}, which does not only affect the way perovskite crystallization is carried out but also provides the composite material with high lead adsorption capacity. Simultaneously, the use of carbon nanotubes facilitates the regulation of the vertical growth of the crystals and the movement of charges in the device, which ultimately increases the efficiency of the battery [10].

4.3. Improve mechanical and thermal stability

Besides the environmental issues, carbon nanotube-based composites also have two important material benefits, high mechanical toughness and high thermal conductivity, which improve the longevity of devices when they are actually operating in various aspects.

To begin with, flexible perovskite solar cells require high flexibility. Compared to brittle transparent electrode materials like ITO, carbon nanotube films are conductive, and also of outstanding mechanical flexibility and strength, allowing them to bend over and over without collapsing. Since perovskite materials have solution-processing properties, this offers a material base of the creation of genuinely flexible, lightweight wearable electronic devices, where potential applications include smart textiles, portable power sources and bendable building-integrated photovoltaic surfaces [11].

Second, outstanding thermal conductivity assists in enhancing the thermal regulation of the device. The carbon nanotube films have very high in plane thermal conductivity, and thus can dissipate localized heat produced during device operation laterally very quickly thus preventing heat buildup and thus conducting away heat through the substrate. This is a very efficient heat diffusion which can greatly eliminate the performance degradation and material damage due to local thermal stress.

On the whole, CNTs incorporation offers numerous protective measures to the practical implementation of PSCs: environmentally, by fixing the lead to minimize the leakage risk; mechanically, by granting the flexibility devices with durability; and thermally, by assisting the devices to remain more stable in the high-temperature conditions. All these advantages demonstrate the essential importance of CNTs to improve the overall reliability of PSCs.

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5. Conclusion

The CNTs because of their high electrical conductivity, tunable energy band structure, excellent chemical stability, and unique one-dimensional morphology have shown that they can be integrated synergistically to achieve more than just single-function use in PSCs. This review article shows that incorporating CNTs into the perovskite active layer as a crystallization regulator can maximize the alignment of the energy levels, simplify the extraction of charges and passivate interface defects; When applied to the encapsulation systems or as an additive, CNTs can very effectively block water and oxygen corrosion, immobilize lead ions, and improve the mechanical and thermal stability of the devices. The multi-layered and multi-functional application strategy promises to be a highly promising systematic approach to the simultaneous resolution of the fundamental issues of perovskite solar cells related to their efficiency, stability, and environmental friendliness.

To conclude, despite the great advances currently achieved in carbon nanotube technology, its commercialization, on large scale, remains a challenging area with concerns being raised on material systems, cost of the process, reliability over time, and knowledge of the fundamental processes. Further studies are needed by creating low-cost, scalable fabrication methods that rely on a more in-depth comprehension of the underlying mechanisms, and the creation of a stability assessment system that is compatible with industrial requirements, and the eventual aim of transferring the carbon nanotube-based perovskite solar cells out of the laboratory and into the real world.

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