Characteristic analysis and comparison of perovskite solar cell

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Abstract: With global warming, energy crisis and other factors, people are in urgent need of finding new energy to replace traditional energy. Solar energy is the most abundant clean energy in the world. Solar cells are one of the effective ways to develop and utilize solar energy. Perovskite solar cells (PSCs) are currently the third generation of new solar cells. Because of their ultra-high absorption coefficient, environmentally friendly and cheap raw materials, and simple spin coating process, they have become a new star in photovoltaic power generation. At present, for the research of perovskite solar cells, this paper hopes to introduce the basic knowledge of perovskite solar cells from a more comprehensive perspective.

Keywords: Perovskite, Third generation, Solar cells, Ionic polarization.

1. Introduction

Perovskite solar cells are solar cells that utilize organic metal halide semiconductors of the perovskite type as light-absorbing components. The third generation of solar cells, commonly referred to as new idea solar cells, includes these solar cells. The greatest efficiency obtained in single-junction silicon solar cells has been surpassed by the solar cell efficiencies of laboratory-scale devices utilizing these materials, which have improved from 3.8 percent in 2009 to 25.7 percent in 2021 and to 29.8 percent in silicon-based tandem cells [1]. Therefore, as of 2016, perovskite solar cells represented the solar technology that was developing the fastest. Perovskite solar cells have gained commercial appeal thanks to their extremely low production costs and promise for even higher efficiency.Their short- and long-term stability are key issues and research topics.

The Shockley-Queisser limit sets a ceiling on the efficiency of solar cells. The theoretical maximum efficiency of a solar cell with a single junction and just radiative recombination within the solar cell is set by this calculation. The highest power conversion efficiency is associated to a certain bandgap based on the AM1.5G global sun spectrum, establishing a parabolic relationship.

There are several research layers on perovskite solar cells since they have the potential to produce improved efficiency and extremely low production costs. This article's goal is to provide future researchers with a reasonably comprehensive overview of the current study findings.

2. Preparation

A preparation method of perovskite solar cell, which is characterized in that it includes the following steps:

(1) cleaning and ozone treatment of the substrate: after scrubbing the substrate with detergent, sputter on one side to generate IT0 film, perform photolithography on IT0 film, cut it to the required size, use IT0 film as a transparent electrode, and then place the substrate in deionized water, ethanol, acetone and deionized water in turn, Ultrasonic cleaning for 10-15 min each time, then blow dry with nitrogen gun, and put the substrate into the ultraviolet ozone machine for ultraviolet ozone treatment for 10-15 min ;

(2) Spin coating of the first transport layer: spin coating a layer of the first transport layer on the surface of the substrate after ozone treatment, controlling the speed of 3000-5000rpm and the time of 40s, and then conducting annealing treatment, controlling the annealing temperature of 90-150 ° C and the annealing time of 20-40min to obtain substrate A;

(3) Preparation of perovskite precursor solution: NH3CH3I and PbI2, PbCl2 or PbBr2 are mixed and dissolved in N, N in a molar ratio of 3:1~1:1_ In dimethylformamide solvent, CH3NH3PbI3, CH3NH3PbI3-xClx or CH3NH3PbI3-xBrx precursor solution is obtained, and then stirred at room temperature for 24h, filtered with 0.45mi organic system filter head to obtain CH3NH3PbI3, CH3NH3PbI3-xClx or CH3NH3PbI3-xBrx precursor solution;

(4) Spin coating of precursor solution: transfer substrate A to the glove box, control the speed at 3000-5000rpm, spin coating time at 30-60s, spin coating a precursor solution on its upper surface, transfer it to the transition chamber, dry it with air extraction for 20-60min, and then place it on the heating plate for annealing. The annealing temperature is 100 ° C, and the annealing time is 60-80min. After the precursor solution is completely crystallized, transfer it to the glass culture dish for cooling, A substrate B containing perovskite thin films is obtained;

(5) Spin coating of the second transport layer: spin coating a second transport layer on the upper surface of substrate B in the glove box, controlling the spin coating speed of 2000-3000rpm and spin coating time of 40s to obtain substrate C;

(6) The introduction of nano light trapping structure on the second transport layer: the substrate C is processed by nano soft embossing process in the glove box, and the substrate D is obtained after the embossing process;

(7) Spin coating of buffer layer: spin coating the solution of interface modification material on the upper surface of substrate D at 4000-6000rpm in the glove box for 40-60s to obtain substrate E;

(8) Evaporation of metal electrode: transfer the substrate E to the thermal evaporation system, and evaporate a layer of silver electrode under the vacuum of 1 Xl (T4Pa). The thickness of the silver electrode is 100-150nm, which is the perovskite solar cell. [2]

3. Structure of perovskite solar cell

3.1 Structure of perovskite

The ideal cell of perovskite (ABX3) is a face centered cubic structure (Figure 1.1), where A, B and X are located at the top corner, body center and face center of the cubic cell respectively. A is a univalent cation, such as Ca, Cs, K, methylamine ions (MA, CH3NH3) and formamidine ions (FA, HC (NH2) 2+); X Usually halogen atoms (I, Br, C) or oxygen atoms; B is a divalent metal cation, such as Pb, Sn, Cr, Ni, Cu and Ti . In addition to face centered cubic cells, perovskite is also displayed as cubic octahedral cells (The cubic structure is shown in Figure 1.), where A is surrounded by twelve Xs to form a cubic octahedral structure.

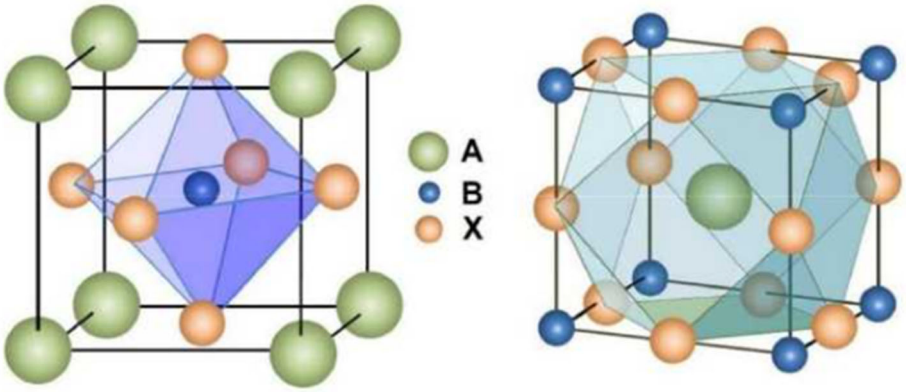

Figure 1. The cubic structure

3.2 Crystal structure of perovskite

The naturally formed perovskite usually exhibits an irregular cubic or quasi cubic phase. If the radius of A ion is too large, the three-dimensional crystal structure of perovskite will be destroyed,

resulting in the disorder of the functional ions. In the process of thin film growth, any structural deviation caused by any factor will change the optical, electrical, magnetic and insulating properties of perovskite. Therefore, perovskite materials commonly used in solar cells, sensors and laser diodes must have stable crystal structures, and their stability is usually determined by the tolerance factor t and octahedral coefficient μ Joint decision 1, the calculation formula is as follows:

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)} \tag{1}$$

$$\mu = {r_B}/{r_X} \tag{2}$$

Where R_A, R_B and R_x are the ionic radii of A, B and X respectively. In general, t and μ Halide perovskite has good stability when it is in the range of 0813-1.107 and 0442-0.895 respectively. When 0.89<1<0.947, the perovskite crystal presents cubic phase. The larger the t is, the narrower the band gap is. If t is too small, irregular tetragonal phase will appear. [3]

PSC initially adopted the liquid electrolyte structure of DSSCS, but the electrolyte will cause rapid dissolution of perovskite crystals. Subsequently, the introduction of solid-state Spio OMETAD transformed the device into an all solid mesoporous structure, but the mesoporous TiO2 in it needs to be sintered at high temperature. Then, the cells developed into planar heterostructure without mesoporous layer. However, With the continuous improvement of the device performance of single junction PSC. Its battery efficiency has gradually approached the maximum efficiency of single crystal silicon battery by 27.6%. At the same time, the commonly used carrier transport layer material is a composite material, which has high process cost. In order to further improve efficiency and reduce cost, some novel battery structures have been proposed, such as: laminated cell structure, gradient band gap structure, carrier free transport layer structure and dual carrier transport layer structure. The design of device structure plays a leading role in the development of PSC, as follows. The research progress of these new structures will be introduced.

3.3 The perovskite laminated battery structure

Laminated battery is an important design concept to break through the Shockley Queiser limit of single junction battery. The perovskite based laminated battery was first prepared by Ballif et al., in which the perovskite is used as the top battery, the monocrystalline silicon c-Si is used as the bottom battery, and the electrical connection is a 4-terminal structure. Although the perovskite top battery cannot contain metal components and presents broadband transparency, but the transmittance of near-infrared light is still lower than 75%, making the efficiency only 13.4% . Subsequently, Buonassisi et al. integrated CH3NH3Pbl3 top cell and c-Si bottom cell by using silicon tunneling junction, simplifying electrical connection and reducing optical loss, and increasing PCE by 0.3% . However, the price of monocrystalline silicon is high, the consumption is large and the production process is complex. To this end, Baie et al. used CIGS as the bottom cell and transparent silver nanowires as the window layer to increase the infrared light transmittance. The efficiency of the stacked cell reached 18.6% . However, the raw materials of CIGS are scarce and have the problem of photo degradation, which also affects the research and application of CIGS as a bottom cell. Based on the low cost, simple process and adjustable band gap width of perovskite materials, a 2-terminal all perovskite laminated battery was designed and studied. In 2015, Im et al. successfully prepared stacked PSC by spin coating method, and its device structure is shown in Figure (a). However, the band gap mismatch (225 eV and 1.55 eV) of broadband gap perovskite Mapbbr3 and narrow band gap perovskite MAPb caused serious current limitation, with current density of only 8.4 mAm3 and efficiency of only 10.8% 1. Subsequently, Snaith et al. used the band gap matching perovskite materials as the intrinsic absorption layers of the top cell and bottom cell respectively to reduce the current limitation. Although the short-circuit current and PCE of the battery were increased to 14.5mA/cm and 17% respectively, the mismatch of energy levels and lattice defects at the interface of NIO/FAO 83 Cs01Pb (Io. s) 3 caused serious recombination loss, resulting in an open circuit voltage of only 166V0. In 2017, American Jen proposed to use the fullerene isomer Bis-C6 ω. To

modify the interface contact, the research shows that Bis-C6 can promote the formation of greater shift of quasi Fermi energy levels and reduce the nonradiative recombination of carriers, so 18.4% PCE-2 is obtained. The battery structure is shown in Figure (b). In 2020, XIao et al. proved that strong reducing zwitterions can improve the homogeneity and stability of narrow band gap perovskite. On the other hand, the zwitterionic antioxidant can not only inhibit the oxidation of Sn+to Sn4, but also passivate the surface defects of the lead tin perovskite film, increasing the efficiency of the laminated perovskite battery to 24.2%. The device structure is shown in Figure 2.

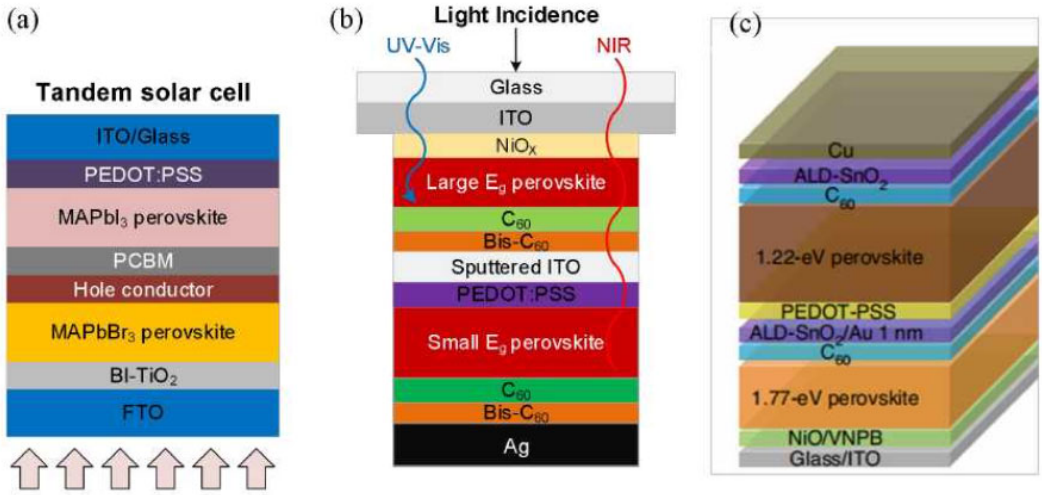

Figure 2. The laminated perovskite battery structure.

3.4 Perovskite graded band gap structure

The experimental results show that the perovskite materials and the commonly used HIL (NiO, Cuscn, Cu, CuO2, PATT, PEDOT PSS) or ETL (TiO2, SnO, ZnO, C '6o) have an irreducible band shift at the heterojunction interface, which hinders the carrier transport and extraction ∞. However, by changing the ratio of organic or inorganic ions, the band gap width of perovskite can be adjusted to 6-38 within the range of 1.17-4.09eV. In order to reduce the energy band offset and enhance the charge transfer, the perovskite graded band gap structure came into being. In 2017, Yin et al. introduced wide band gap CSPBBIXI3x as HTL to replace Spio OMETAD to adjust the band gap gradient by changing the B ratio. It is found that the gradient band gap can promote the transmission of photogenerated charges, reduce the surface recombination of carriers at the perovskite Au interface and enhance the stability. However, the intrinsic CSPBBIXI3x does not form enough built-in electric field with MAPBI to enhance charge extraction, the current density is only 17.69mAcm °, and the efficiency is only 113% - 9. Subsequently, Liu et al. combined Cspb Br and Cspb3 quantum dots into gradient band gap perovskite (as shown in Figure 1.6), and reduced the lattice defects of gradient band gap cells through Cs+interface modification, increasing the efficiency to 14.45% . In the same year, Zhang exchanged Br and I ions in MAPBI3-XBIX in situ through thermal evaporation, forming a perovskite material with increasing band gap, which prevented the diffusion of photogenerated holes to the cathode, and also made the perovskite self passivated. The electronic life was improved to 100s, and the efficiency was increased to 16.6% . In addition, Fu et al. also prepared gradient perovskite films by ion exchange method, and obtained 16.8% PCE . Up to now, the highest efficiency of gradient band gap PSC is 21.7%, which is reported by Ergen et al. By adjusting the concentration of PbSn and b ions to change the band gap gradient, and using Gan to enhance electron injection, graphene gel promotes surface crystallization.

It is found that 2D perovskite material formed by inserting larger cations into 3D MAPBI3 lattice can significantly enhance the humidity resistance of the film and improve the stability of the device. In 2014, Smith research group introduced PEA+(CH5 (CH2) NH3) into Mapi3 lattice to prepare 2D

perovskite (PEA) 2 (MA) [PbI, thin films show high density. The perovskite materials are exposed to 52% humidity, and PCE does not decay after 46 hours. However, the perovskite films without 2D materials decay after 4 hours. This proves that 2D perovskite materials have the ability to improve stability. 8 The stability of perovskite is closely related to various ions of the lattice structure ABX3. Amat et al. found that the force between FA and surrounding octahedral PbI is stronger than that of MA+1 under light. MAPBI3 There are many degradation mechanisms, one of which is that the H ions released by MA+and I form hydroiodic acid (HI). Due to the resonance characteristics of FA+through CN bond, FA+releases much less H ions than MA. Therefore, compared with MAPBI3, Fabbi3 have better light stability. In addition, Fabbi3 exhibits lower sensitivity than MAPI3 at high temperatures. Subsequently, the researchers partially replaced FA+with Cs+to obtain more stable FAO gcso Pbi383]. In 2017, Saliba et al. reported that the perovskite material CSz (MA1FA083) axPb (Io3Bro1n) 3 based on three cation Cst+MA+FA+has higher stability, and the PCE is still as high as 21.1% after 250 hours of storage. In addition, Gratzel et al. doped Rb into trication perovskite to form tetracation perovskite. The stability was again improved, and 21.6% efficiency was obtained (s. In addition to A+ions, metal B+ions are also crucial to the structural stability of perovskite. Pb is a commonly used B ion. However, Pb is toxic, which will seriously affect the environment and health. Research reports that using Sn instead of Pb will lead to a decrease in lattice stability. Because Sn Hung - is easy to be oxidized to more stable S φ To destroy the crystal structure. Up to now, the stability of Pb free PSC is still poor, which needs further research. At the same time, the influence of halogen atoms (Cl, Br and D) on the stability of perovskite is also discussed. Seok et al. used Br to partially replace I. When the ratio of B was 1:4, MAPb (Io. abro.) 3 did not attenuate after 20 days, proving better stability. Subsequently, Zhao et al. found that the introduction of some Cl atoms can improve the crystallinity of the film and provide better stability. The above shows that the stability of perovskite thin films can be improved by introducing FA, Cs, Rb, Br and l ions with appropriate concentrations. However, excessive doping may lead to a decline in stability.

4. Conclusion

Due to its high absorption coefficient, low exciton binding energy, long carrier diffusion length, and low defect state density, perovskite materials have received a lot of interest recently. The photoelectric conversion efficiency of perovskite solar cells (PSCs) has rapidly improved from 3.8 percent to more than 25 percent after more than 10 years of development, achieving a level of performance equivalent to that of commercial polysilicon solar cells. The preparation of solar cells and the perovskite crystal structure are discussed in this paper as an introduction to the development of perovskite solar cells. Despite the foregoing benefits, there is still significant opportunity for advancement in perovskite solar cells on the commercial front.

Under environmental conditions including water, temperature, and oxygen, the perovskite absorption layer is easily broken down. Perovskite absorption layer is easy to decompose under environmental factors such as water, temperature, oxygen and ultraviolet light, which leads to the decline of long-term stability of PSCs and seriously restricts its commercial application. Therefore, it is urgent to improve the stability of perovskite absorption layer, so as to build a stable PSCs device.

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