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تاثیر برم بر روی پروسکایت ترکیب هالوژنی

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چکیده

سلول خورشیدی پروسکایتی ترکیب هالوژنی با روش لایه نشانی دو مرحله‌ای پروسکایت معرفی می‌شود. سرب و ید از پیش ماده سرب یدید و برم از پیش ماده متیل آمونیوم برماید تهیه می‌شود. تاثیر برم روی ولتاژ مدار باز و گاف انرژی سلول خورشیدی نشان داده می‌شود. افزودن برم به پروسکایت یدی باعث بهبود مورفولوژی سطح و پهن‌تر شدن گاف انرژی پروسکایت و در نتیجه افزایش ولتاژ مدار باز سلول خورشیدی حاصل می‌شود. اما، بروم با متخلخل کردن ساختار پروسکایت، باعث کاهش جریان اتصال کوتاه سلول می‌شود. آنالیزجذب فرابنفش-مرئی نشان می‌دهد این ساختار پروسکایت دو گاف انرژی دارد. به عبارت دیگر پروسکایت حاصل دوفازی است.

کلید واژه: سلول خورشیدی، پروسکایت، متیل آمونیوم برماید، ولتاژ مدار باز، جریان اتصال کوتاه.

The effect of bromine on the mixed halide perovskite

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Abstract

Using the sequential deposition method, we introduce a mix halide perovskite solar cell. The Pb and I are provided by PbI_2 precursor and Br is delivered by Methyl ammonium bromide (MABr) precursor. The effect of Br on the open circuit voltage (V_{OC}) and the band gap is studied. Addition of Br to the iodide-based perovskite improves its surface morphology and widens the perovskite bandgap, and hence increases the resulting solar cell V_{OC}. However, pinholes created in the perovskite layer due to addition Br results in a dramatically reduced short circuit current density (J_{SC}). The UV-Vis spectroscopy, indicating two optical bandgaps, confirms a two-phase perovskite structure is produced.

Keywords: Keywords: Solar cell, perovskite, MABr, open circuit voltage, short circuit current.

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1 Introduction

In general, the low cost, low power consumption, and high light absorption are very important challenges in the solar cells technology. [1],[2],[3],[4]
Perovskite-based solar cells (PSCs) have the potential to overcome these fundamental challenges. The discovery of perovskite materials has improved the solar-energy conversion because of their extraordinary optoelectronic characteristics such as long diffusion lengths, low recombination rate, high light absorption coefficient and tunable band gap.[5] In the primary of perovskite solar cells, the reported power conversion efficiency (PCE) was 3.8. With the extensive study of perovskite (PSK) the crystalline structure of this material has improved, and recently, a pinhole free perovskite layer has achieved. [2],[4] The highest power conversion efficiency obtained for the perovskite solar cells is 22.7%. [6]
In this research, we have studied the effect of bromine on the morphology and the grain size of PSK. Also, we have considered the impact of mixed halide precursors (i.e. Br and I) on the photovoltaic performance of PSCs. [5],[7],[8] We have confirmed that V_{OC} has increased due to increasing the band gap. When the iodide-based perovskite doped with Br content, short circuit current has decreased influenced by the pinholes in the perovskite structure. The mixed halide perovskite-based solar cells have a desirable stability.
At the previous work, halogen ions (i.e. Br and Cl) doped the perovskite layer for tuning the band gap and increasing the V_{OC}. [9],[10],[11],[12] The surface coverage and morphology of thin film PSK very impressed with deposition methods. In this work, we have prepared perovskite layer via sequential two-step deposition. [7], [8]

2 Perovskite Preparation

We have spin-coated the perovskite layer with the sequential deposition method that improves the stability and optical and electronic properties of the photo-absorbing layer. Figure 1 shows the two-step deposition method for the formation of $CH_3NH_3PbI_{3-x}Br_x$ thin film perovskite. [8]

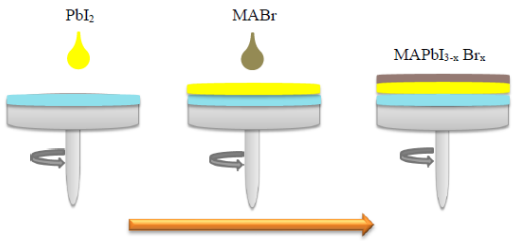

Figure 1: Schematic of sequential spin-coating for the $CH_3NH_3PbI_{3-x}Br_x$ based perovskite layer.

In this method, first, we have deposited the PbI_2 solution on top of the mesoporous TiO_2 followed by annealing the film on the hotplate. Then, we have deposited the bromide solution (i.e., MABr) on top of the PbI_2 surface and annealed again on the hot plate to form a dark perovskite film (Fig 1).

3 Result and Discussion

Figure 2 shows the absorption spectra of deposited thin film PSK as measured with UV-vis spectroscopy. We have measured the optical band gaps of $CH_3NH_3PbI_{3-x}Br_x$ which are larger than the

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previously reported value for the iodine-based perovskite layer. The $CH_3NH_3PbI_{3-x}Br_x$ perovskite layer has shown two absorbance edges and two band gaps.
Appearing two absorbance edges evoke formation of the two-phase crystalline structure of perovskite. In the growth of the perovskite structure, Br atoms could place in the perovskite structure so the mixed halide perovskite structure has formed.

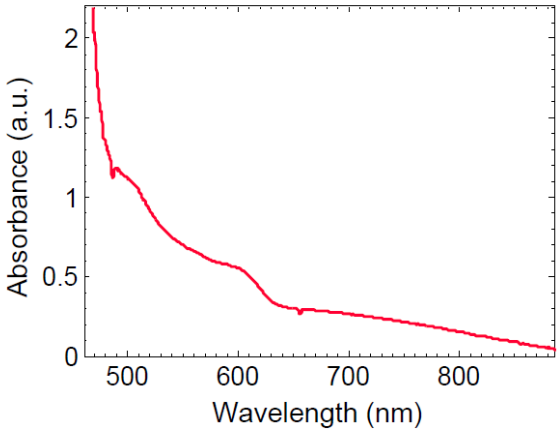

Figure 2: The perovskite absorption spectrum.

The X-ray diffraction pattern, which agrees well with the previous statement for the absorbance spectra. It proves a validation that the sequential deposition process successfully produces two-phase perovskite. Figure 3 shows the obvious $CH_3NH_3PbI_{3-x}Br_x$ based perovskite main peak. The main peak of perovskite appearances at the 14.52°. The main peak appearance at the 14.02° for the iodide-based perovskite. The shift in the perovskite peak has illustrated that Br ions have incorporated in the crystal structure. In additional, diffraction

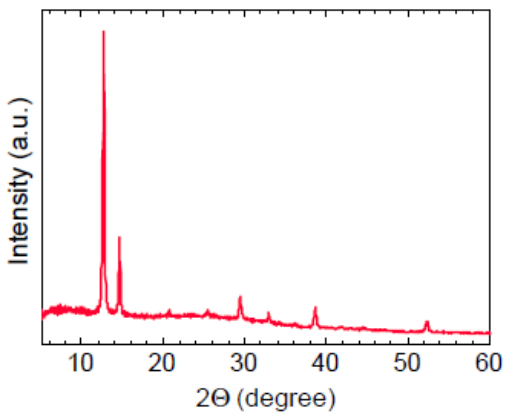

Figure 3: XRD graph for $MAPbI_{3-x}Br_x$ perovskite.

peaks show the PbI_2 peak (2θ ≈ 12.7°) clearly. This PbI2 peak may identify that the some of the iodide precursors have converted to the perovskite phase.
The open circuit voltage (V_{OC}) increases for the $CH_3NH_3PbI_{3-x}Br_x$ based perovskite devices. Figure 4 shows the J-V characteristics of devices. Table 1 presents the performance of the best PSCs obtained from MABr precursor. We can see easily that the presence of Br ions in the perovskite precursor have increased the open circuit voltage due to increasing the bandgap of perovskite photo-absorber layer.
However the two-phase perovskite grains size has decreased and grain boundaries and pinholes have increased (Fig 5) therefore the bromide mixed halide perovskite-based cell has very low current density. Also, the power conversion efficiency and fill factor (FF) for this cell don't have significant amounts.
Regarding the FE-SEM image demonstrates that the presence of relatively large pin-holes in the perovskite layer has increased the recombination of the carriers resulting in a drop in current density.

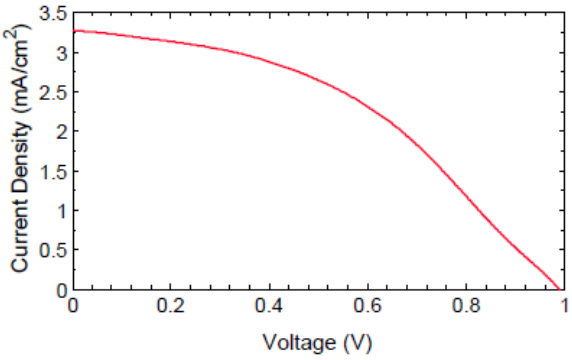

Figure 4: *J–V* characteristic of solar cell based on $MAPbI_{3-x}Br_x$ perovskite.

Figure 5 exhibits the FE-SEM image of perovskite layer. The morphology of perovskite is not uniform so many defect states have trapped electrons and holes carriers. The perovskite structure has contained pinholes which have increased recombination centers and can decline device performances dramatically.

Table 1: Device performance parameters

Cell	V_{OC}	J_{SC}	FF	PCE
$MAPbI_{3-x}Br_x$	0.99	3.27	0.43	1.39%

Tandem structures have been introducing recently that can provide the efficient solar cells with the high light absorption capacity and high power

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conversion efficiency. The $CH_3NH_3PbI_{3-x}Br_x$ based perovskite layer can use for the tandem structure.

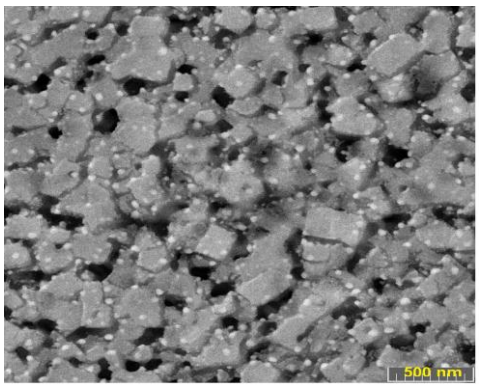

Figure 5: SEM image of $MAPbI_{3-x}Br_x$ perovskite layer grown on the TiO_2 mesoporous scaffold layer.

4 Conclusion

In this work, we introduced a mixed halide perovskite thin film and the effect of Br incorporation in the fabrication of the perovskite solar cells. We used the methylammonium bromide composition in the growth of perovskite layer. The XRD and UV-Vis spectroscopy analysis confirmed the formation of a two-phase perovskite structure. Addition of Br to the $MAPbI_3$ perovskite resulting in $MAPbI_{3-x}Br_x$ with an improved surface morphology but wider bandgap. Although this increases the resulting solar cell V_{OC}, the pin holes created in the perovskite by Br reduces J_{SC}, dramatically.

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