مطالعه استحاله ساختاری پروسکایت های ترکیب هالوژنی

فرزاد مرده‌کتانی اصل[۱]، زهرا یگانگی[۱]، بهرام عبداللهی نژند[۱،۲] و محمدکاظم مروج فرشی[۱]

۱ دانشگاه تربیت مدرس، دانشکده مهندسی برق و کامپیوتر

[۲] جهاد دانشگاهی تربیت مدرس، گروه تکنولوژی نانوذرات

چکیده – مواد پروسکایتی به واسطه خواص اپتوالکترونیکی خارق‌العاده‌ای که دارند، در طی سال‌های اخیر مورد توجه بسیاری قرار گرفته‌اند. علی‌رغم پیشرفت‌های فراوان در زمینه ساخت سلول‌های خورشیدی پروسکایتی با بازده بالا، همچنان ابهامات فراوانی در مورد نحوه عملکرد آنها وجود دارد. یکی از مهمترین مشکلات سلولهای خورشیدی پروسکایتی پایداری طولانی مدت این مواد است. در این پژوهش نحوه تشکیل پروسکایت با استفاده از دو پیش ماده یدید سرب و متیل آمونیوم کلرید بررسی شده‌است. یدید سرب با استفاده از روش لایه نشانی دورانی رایج در روش‌های چند مرحله‌ای لایه نشانی شده‌است. در مرحله بعدی این پیش ماده در معرض ماده متیل آمونیوم کلرید در زمان‌های مختلف قرار گرفته‌است. نتایج به دست آمده با روش‌های مشخصه‌یابی الگوی پراش اشعه ایکس و همچنین طیف جذب نوری، نشان دهنده تغییر مواد تشکیل شده در زمان‌های متفاوت است.

کلید واژه- پروسکایت، سلول خورشیدی، استحاله ساختاری، روش چند مرحله ای

Study of Structural Phase Transformation in Halide Pervoskites

Farzad Mardekatani Asl[1], Zahra Yeganegi[1], Bahram Abolladhi-Nejand[1, 2] and Mohammad Kazem Moravvej-Farshi[1]

1 School of Electrical and Computer Engineering, Tarbiat Modares University, Tehran-Iran

2 Nanomaterial Research Group, Academic Center for Education, Culture and Research (ACECR) on TMU, Tehran, Iran

Abstract- Perovskite materials have gained a lot of attention because of their extraordinary optoelectronics properties. Solarcells based on these materials have reached power conversion efficiency of above 20% in a short period of time. However, there has still work to do about their stability and durability. In this work we demonstrate the effect of CH_3NH_3Cl on PbI_2 to produce a perovskite layer. PbI_2 , the first precursor, was deposited using common spin coating method mentioned in the literature. The deposited layer was exposed to CH_3NH_3Cl solution. XRD and UV-Visible characterizations were done. The devices fabricated using this layers have shown power conversion efficiency of 5.4%.

Keywords: Solar cells, Perovskites, Sequential deposition, Phase transformation

[Downloaded from www.opsi.ir on 2026-11-01]

This paper is authentic if it can be found in www.opsi.ir.

Study of Structural Phase Transformation in Halide Pervoskites

Farzad Mardekatani Asl	Zahra Yeganegi	Bahram Abollahi-Nejand	Mohammad Kazem Moravvej-Farshi
fmardekatani@modares.ac.ir	zhr.yegane@modares.ac.ir	b.abdollahi@modares.ac.ir	

1 Introduction

Metal Halide perovskites due to their excellent optoelectronics properties have emerged as a potential absorber layer for thin film solar cells[1]–[3]. Their high carrier mobility and high optical absorption are the main reasons of their excellent photovoltaic properties[4], [5]. Solar cells fabricated using perovskite materials have reached the efficiencies above 20% recently[6]. Moreover the main advantages of these materials over other photovoltaic technologies are their low cost and facile deposition methods[5], [7]. But still, they lack a long durability and also presence of lead in their structure has caused environmental concerns[5], [8].

Methyl ammonium lead triiodide ($MAPbI_3$) is the main perovskite material that is used as light absorber for solar cells[5], [9]. Mixed halide perovskites are also used to tune the bandgap and durability of fabricated devices and [10]–[12]. Bromine as another halide has been added to the structure of perovskite[10]. Increased bandgap in comparison to $MAPbI_3$ is the first consequence of adding bromine in the perovskite structure[10]. Another effect of bromine is increasing the stability of perovskite structure. It has been shown by Noh and et al that perovskites with a certain amount of bromine in their structure are more resistant to humidity and other environmental effects[10].

But chlorine as another halide has a different behaviour in perovskite structure. The first solar cell using perovskite as light absorber in the work of Snaith and co-workers, used $MAPbI_{3-x}Cl_x$ [11]. Later studies on $MAPbI_{3-}xClx$ have showed a diffusion length longer than 1μm[4]. Yang and co-workers showed that chlorine is escaping the structure during the formation on perovskite layer and it only helps to enlarge the grain boundaries [13].

In this work, we have used methyl ammonium chloride (MACl) to convert PbI_2 to perovskite layer. Perovskite layers showed a two phase structure at short times of dipping but for the long times a single phase structure of mixed halide perovskite is fabricated. The best cell fabricated using this method showed a power conversion efficiency (PCE) of 5.4%

.

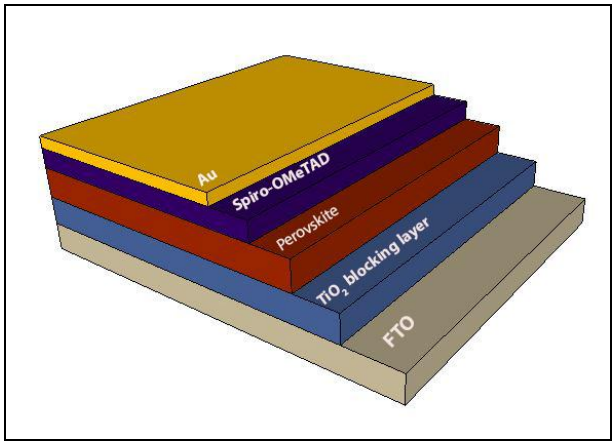


Figure 1: Fabricated device structure

2 Experimental Details

2.1 Preparing compact layer

FTO-coated glass substrates were patterned by Zn powder and 2M HCl solution etching. The

This paper is authentic if it can be found in www.opsi.ir.

[Downloaded from www.opsi.ir on 2026-11-01]

patterned FTO substrates were cleaned by soap-deionized water solution, followed by ultrasonication at 50℃ deionized water, ethanol, and isopropanol, and then subject to an O_3/ultraviolet treatment for 20 min to room temperature. First a ltc-TiO_2 deposited on FTO and after treated with 200mM $TiCl_4$ at 70° C for 20 minutes[14].

2.2 Deposition of perovskite layer

PbI_2 layer was deposited by spin coating of 1.25M solution of PbI_2 in *N*,*N*-dimethylformamide (DMF). The layers are dipped into a MACl precursor with a concentration of 10mg/mL for different times. It is followed by a thermal annealing of 100° C on a hotplate for 10 minutes.

2.3 Deposition of Spiro-OMeTAD/Au

Spiro-OMeTAD-based hole transporting layer was deposited using preparation method mentioned in previous works [9]. Au as a back contact was deposited by thermal evaporation. The fabricated layer is 100nm thick.

3 Results and Discussion

Fabricating perovskite layer with the sequential steps method is a well-known and common method to produce a uniform and low pin-hole layer[3]. In this regard, we used MACl for the second precursor to convert the first precursor to perovskite.
Fabricated perovskite layer in the first time due to the figure 2 has shown a two phase structure. We can see in the XRD results that there are two peaks for perovskite layer. One in 14.1 for the $MAPbI_3$ and one in 15.6 for the mixed perovskite layer. But as we increase the dipping time the peak relating to $MAPbI_3$ is disappearing. Moreover, the main peak in the 12.6 is related to remained PbI_2 layer. But as shown in figure 2(black curve), by increasing the time of dipping all the PbI_2 is converted to perovskite. XRD results also indicate a high crystalline mixed perovskite layer.

One of the main characteristics for absorber layers in solar cells are their absorption spectrum. $MAPbI_3$ absorbs light from 1.55 eV photon energy and higher[15]. Fabricated perovskite layers have shown two absorption onset, indicating their two phase structure.

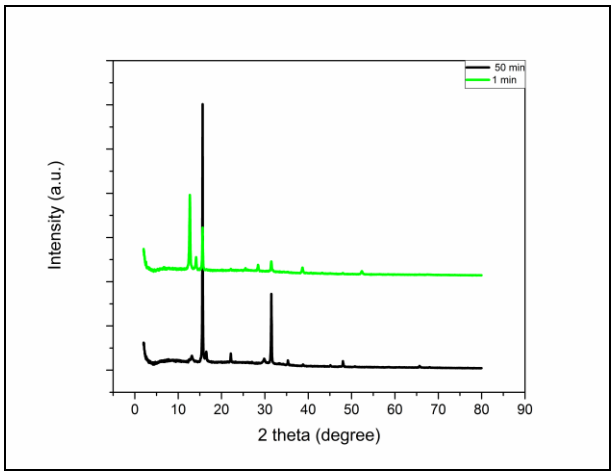


Figure 2: XRD measurement for fabricated layers

Figure 3 shows the absorption spectrum of the deposited layers.

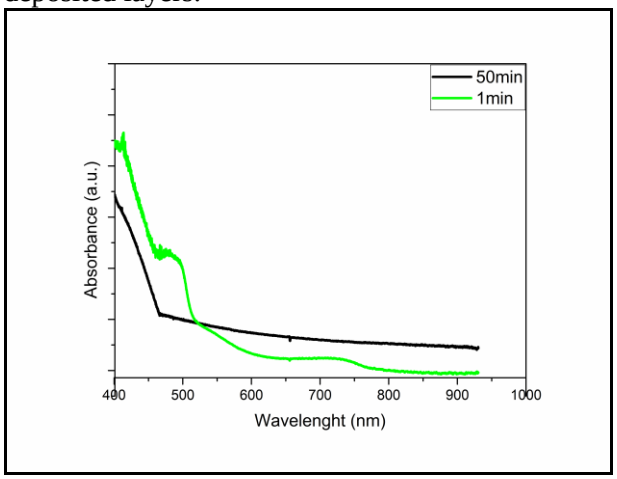


Figure 3: UV-Visible spectrum for fabricated layers

Fabricated devices using the two phase perovskite layers with the normal device architecture, has reached a PCE of 5.4% and open circuit voltage of 1.02 volts.

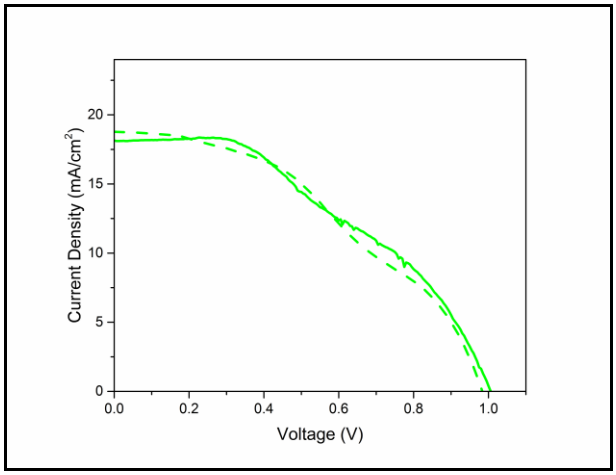


Figure 4: J-V measurements of fabricated devices (dashed line shows the reverse scan)

4 Conclusion

This paper is authentic if it can be found in www.opsi.ir.

[Downloaded from www.opsi.ir on 2026-11-01]

A sequential method with a new second precursor was studied. For short periods of dipping in second precursor a two phase perovskite structure was fabricated. As we increased the time of dipping the $MAPbI_3$ disappeared.
Devices fabricated using the two phase perovskite layer has shown a PCE of 5.4% and open circuit voltage of 1.02 volts.

Acknowledgements

The authors would like to thank NOPL for the equipment and Mr Masoud Payandeh for technical help and constructive discussions.

References

[1] M. M. Lee, J. Teuscher, T. Miyasaka, T. N. Murakami, and H. J. Snaith, "Efficient Hybrid Solar Cells Based on Meso-Superstructured Organometal Halide Perovskites," *Science (80-.).*, vol. 338, no. 6107, pp. 643–647, Nov. 2012.

[2] M. Liu, M. B. Johnston, and H. J. Snaith, "Efficient planar heterojunction perovskite solar cells by vapour deposition," *Nature*, vol. 501, no. 7467, pp. 395–398, 2013.

[3] J. Burschka *et al.*, "Sequential deposition as a route to high-performance perovskite-sensitized solar cells," *Nature*, vol. 499, no. 7458, pp. 316–319, Jul. 2013.

[4] S. D. Stranks *et al.*, "Electron-Hole Diffusion Lengths Exceeding 1 Micrometer in an Organometal Trihalide Perovskite Absorber," *Science (80-.).*, vol. 342, no. 6156, pp. 341–344, Oct. 2013.

[5] S. Shi, Y. Li, X. Li, and H. Wang, "Advancements in all-solid-state hybrid solar cells based on organometal halide perovskites," *Mater. Horiz.*, vol. 2, no. 4, pp. 378–405, 2015.

[6] M. Saliba *et al.*, "Cesium-containing triple cation perovskite solar cells: improved stability, reproducibility and high efficiency," *Energy Environ. Sci.*, vol. 9, no. 6, pp. 1989–1997, 2016.

[7] P. Nazari, F. Ansari, B. Abdollahi Nejand, V. Ahmadi, M. Payandeh, and M. Salavati-Niasari, "Physicochemical Interface Engineering of CuI/Cu as Advanced Potential Hole-Transporting Materials/Metal Contact Couples in Hysteresis-Free Ultralow-Cost and Large-Area Perovskite Solar Cells," *J. Phys. Chem. C*, vol. 121, no. 40, pp. 21935–21944, Oct. 2017.

[8] F. Giustino and H. J. Snaith, "Toward Lead-Free Perovskite Solar Cells," *ACS Energy Lett.*, vol. 1, no. 6, pp. 1233–1240, Dec. 2016.

[9] J.-H. Im, I.-H. Jang, N. Pellet, M. Grätzel, and N.-G. Park, "Growth of CH3NH3PbI3 cuboids with controlled size for high-efficiency perovskite solar cells," *Nat. Nanotechnol.*, vol. 9, no. 11, pp. 927–932, Aug. 2014.

[10] J. H. Noh, S. H. Im, J. H. Heo, T. N. Mandal, and S. Il Seok, "Chemical Management for Colorful, Efficient, and Stable Inorganic–Organic Hybrid Nanostructured Solar Cells," *Nano Lett.*, vol. 13, no. 4, pp. 1764–1769, Apr. 2013.

[11] M. M. Lee, J. Teuscher, T. Miyasaka, T. N. Murakami, and H. J. Snaith, "Efficient Hybrid Solar Cells Based on Meso-Superstructured Organometal Halide Perovskites," *Science (80-.).*, vol. 338, no. 6107, pp. 643–647, Nov. 2012.

[12] S. A. Kulkarni, T. Baikie, P. P. Boix, N. Yantara, N. Mathews, and S. Mhaisalkar, "Band-gap tuning of lead halide perovskites using a sequential deposition process," *J. Mater. Chem. A*, vol. 2, no. 24, pp. 9221–9225, 2014.

[13] Q. Chen *et al.*, "The optoelectronic role of chlorine in CH3NH3PbI3(Cl)-based perovskite solar cells," *Nat. Commun.*, vol. 6, pp. 1–9, 2015.

[14] Z. Liu *et al.*, "Low-Temperature TiO x Compact Layer for Planar Heterojunction Perovskite Solar Cells," *ACS Appl. Mater. Interfaces*, vol. 8, no. 17, pp. 11076–11083, May 2016.

[15] W.-J. Yin, J.-H. Yang, J. Kang, Y. Yan, and S. Wei, "Halide perovskite materials for solar cells: a theoretical review," *J. Mater. Chem. A*, vol. 3, no. 17, pp. 8926–8942, 2015.

[Downloaded from www.opsi.ir on 2026-11-01]

This paper is authentic if it can be found in www.opsi.ir.