Molecular Assay of Structural Phase Transformation in Halide Perovskites

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Abstract- Perovskite materials have gained a lot of attention because of their extraordinary optoelectronics properties. Solar cells based on these materials have reached power conversion efficiency of above 20% in a short period of time. However, there is 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 these layers have shown power conversion efficiency of 5.4%.

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

Study of Structural Phase Transformation in Halide Perovskites

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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$_3$-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%.

![Fabricated device structure](image)

2 Experimental Details

2.1 Preparing compact layer

FTO-coated glass substrates were patterned by Zn powder and 2M HCl solution etching. The
patterned FTO substrates were cleaned by soap-deionized water solution, followed by ultrasonication at 50°C deionized water, ethanol, and isopropanol, and then subject to an O₃/ultraviolet treatment for 20 min to room temperature. First a lt-c-TiO₂ deposited on FTO and after treated with 200mM TiCl₄ at 70°C for 20 minutes[14].

2.2 Deposition of perovskite layer

PbI₂ layer was deposited by spin coating of 1.25M solution of PbI₂ 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 MAPbI₃ and one in 15.6 for the mixed perovskite layer. But as we increase the dipping time the peak relating to MAPbI₃ is disappearing. Moreover, the main peak in the 12.6 is related to remained PbI₂ layer. But as shown in figure 2(black curve), by increasing the time of dipping all the PbI₂ 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. MAPbI₃ absorbs light from 1.55 eV photon energy and higher[15]. Fabricated perovskite layers have shown two absorption onset, indicating their two phase structure.

4 Conclusion
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.

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**References**


