Investigation the Effect of Chemical Composition of Perovskite Layer on Performance of Perovskite Solar Cells

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ABSTRACT: In this work, a modest method for creating Perovskite solar cells (PSCs) by recycling car batteries is used. Trying to get rid of some structures or materials which are harm to the environment. However, by reusing car batteries we will avoid the disposal of toxic battery materials and provide an alternative technique, readily-available Pb source for fabricating PSCs. Perovskite solar cells (PSCs) were prepared by two-step spin coating solution method on the FTO glass substrate. Lead iodide (PbI_2) and methyl-ammonum iodide (CH_3NH_3I) used to form the structure of the precursor ($CH_3NH_3PbI_3$). The photovoltaic performance of PSCs and the effect of chemical composition of perovskite layer on performance of PSCs was investigated. Characterization of PSCs by using X-ray diffraction, SEM and the effect of chemical composition on of MAPI films was achieved. It was found that the thickness ratio of (PbI_2/MAI) with 3.0:1 have highest fill factor and maximum efficiency.

KEYWORDS: **Perovskite, Chemical Composition, Photocells, Efficiency, Fill Factor.**

I. INTRODUCTION

Perovskite solar cells (PSCs) halide perovskite organic-inorganic solar cells have attracted a great deal of attention of solar cell research community due to an incredible device efficiency improvement from 3.8% to22.1% since 2009 [1-2]. PSCs not only solve energy crisis, also reduce the emission of CO2 causes the global warming and eradicating of toxic lead in old car batteries for serving solar energy. The PSCs resources need established through mainly The band gap of the thin active Perovskite layer ($CH_3NH_3PbX_3$) is (1.5 eV to 2.3 eV) [3],with a high light absorption coefficient more than (10^4 cm^{-1}) [4-5] which is like other CdTe [6] and copper zinc tin sulphide [7] to other thin film solar cells. Its low-cost and suitable construction methods similarly help as the likely compensations over plan of silicon-base that need complicated and high-vacuum statement approaches. The study of cell production on the stable uniformity of materials has opened up the best opportunities for critical PSCs designed from rolls to allow containers to be discarded in the industry [8-10].The early sense of perovskite was around the mineral crystal of ($CaTiO_3$), The German mineralogist Gustav Rose was discovered in 1839 and named the Russian mineralogist Lev Perovskite [7]. The term perovskite is mentioned in all mixtures with the same mineral composition as $CaTiO_3$. PRK solar cells are the general principle of ABX3 in light-absorbing films, anywhere A is organic cation part example $CH_3NH_3^+$, B is a part of metallic cation for example lead and X anions of the anion halide such as iodide (I−). PRK materials have a common crystalline structure, described as ABX_3, where A and B are cations with different sizes, and X is an anion. Organic cation (such as methyl ammonium $CH_3NH_3^+$, ethyl ammonium $CH_3CH_2NH_3^+$, methyl ammonium $NH_2CH= NH_2^+$), The organometallic PRK halide is a cation of a metal of the carbon group (e.g., Ge_2^+, Sn_2^+, Pb_2^+) and a halogen anion (i.e., F-, Cl-, Br-, I-). methyl ammonium lead iodide ($MAPbI_3$) are the most commonly used light-absorbing layers. Due to concerns about the dangers of lead in method formation, some new works have identified a method for exchanging lead with new metal ions, especially important future development methods [11-12], several halide anions (Br−, I− and Cl−), organic cations ($NH_2CH=NH_2^+$ and $CH_3NH_3^+$), and inorganic cations (Sn_2^+ and Cs_2^+) have been used to advance the effectiveness and constancy. The Perovskite has different levels of structure depending on the change in temperature. When the temperature is below 100 K, the unit cell structure will have an orthorhombic phase. When the temperature rose to 160 K, the tetragonal phase (β) became visible and replaced the peculiar orthogonal phase (γ) [13]. With a further increase in temperature of about 330 K, the tetragonal phase was replaced by other unchanged cubic (α) phases [14]. Here the chemical composition on $CH_3NH_3PbI_3$ active layer has been investigated and the efficiency of the fabricated device was measured using light source of AM1.5- illumination [light intensity of 100 mW cm^2]. The morphology and thickness of PSCs were characterized using scanning electron microscopy (SEM) (Model: JSM-7600 F, Jeol). X-ray diffraction (XRD) technique (Rigaku ATX-XRD) with Cu Ka radiation (k = 1.5405 Å.

II. METHODOLOGY

Harvesting material from the anodes and cathodes of car battery due to separate the car battery (12 V ,799.7gm lead) with metallic harvester [15].The electrolyte acid was emptied out and prudently composed, and the electrodes in addition to the inner barrier of car battery were cleaned some periods by much clean water. The dry car battery was then removed from the top cover, and then fractions of the electrode boards were visible from the sides. After steaming, the substances obtained from lead were separated from modern storage rings by lead (anode) and lead dioxide (cathode) and subsequently wiped with dilute hydrochloric acid and gradual water. Prefix the ingredients together for greater mixing. Lead dioxide (PbO2) can be used in a muffle furnace using a ceramic crucible by converting lead dioxide to lead oxide (PbO) and burning at 600 ° C for 5 hours, after heating it must be cooled to room temperature. The color was from dark brown to yellow color. Preparation of lead iodide from lead nitrate by continuous stirring in a magnetic stirrer 3g of Pb in 5 ml of nitric acid. Dissolve (lead), get lead iodide from lead acetate, dissolve 3 g of PbO (lead oxide) in 5 ml of acetic acid. Then 10 mL of potassium iodide is dissolved, potassium iodide is a catalyst to increase the reaction rate. Mix the solution [SOL] for 30 minutes at 500 rpm using magnetic stirrer. Run the solution under aerobic conditions for 1 day, then filter the result using a centrifugal motor. The SOL should be entrained in a centrifuge cylinder, then add deionized water to the SOL, then centrifuge the SOL at 5000 rpm for 5 minutes, repeat the process 3 times to completely remove the acid concentrate, in the condensed form. Precipitation will slow down, then acid precautions need to be removed. After centrifugation, the SOL must be dried under aerobic conditions, through this process the SOL must be placed in a fume hood. Then to Preparation of methylammonium iodide (CH_3NH_3I) Firstly, HI (Sigma-Aldrich ($\#210021 - 50\,\mathrm{ML}$, 99.95%) was mixed with Methylamine (CH_3NH_2) in methanol and enthused in ice bath till white crystals were molded. Secondly, methanol was unconcerned then the result and filtrated to prepare white crystals of CH_3NH_3I.The organo-halide PRK solar cell consists of five layers to form the first layer of PSC using an FTO glass substrate. The FTO glass should be prepared with IPA (isopropyl alcohol) by leaving it in IPA (isopropyl alcohol) for 30 minutes. And used ohmmeter to know the conductive side. A 150 nm thick electron transport layer (ETL) is used to produce cells from TiO_2 deposited by spin coating process. Method at 3000 r.p.m. coated on the conductor face of FTO glass substrate. The thick MAPI film deposited by this method is called the two-step sequential method [16] the PbI_2/MAI thickness ratio varing from 1.5:1,2.6:1,3.0:1 and 4.5:1 at room temperature. A 100 nm thick hole transport layer (HTL) of copper iodide (CuI), deposited by centrifugation, and an 80 nm thick Ag layer used as an anode, and thermally vaporized, deposited on top of the device. Thermal evaporation was achieved at a base pressure of 10^{-5} mbar.More details about methodology for PSC fabricating, or preparation of chemicals materials [17].

III. RESULT AND DISCUSSION

3.1 Analyzing the film's structure

The effect of chemical composition (determined from the thickness ration PbI_2/MAI) on the phase, structure and microstructure of MAPI thin films by XRD measurements. XRD spectra of MAPI films prepared varying the chemical composition, are showed in Figure 1. that examples deposited with excess of MAI (ratio 1.5:1) present a mixture of the phases MAPI, MAI, and PbI2, while those with excess of PbI_2 (ratio 4.5:1 and 3:1) grow with a mixture of the phases MAPI and PbI_2. However, we were able to grow samples of MAPI free of new phases using a PbI_2/MAI thickness ratio close to 2.6:1.

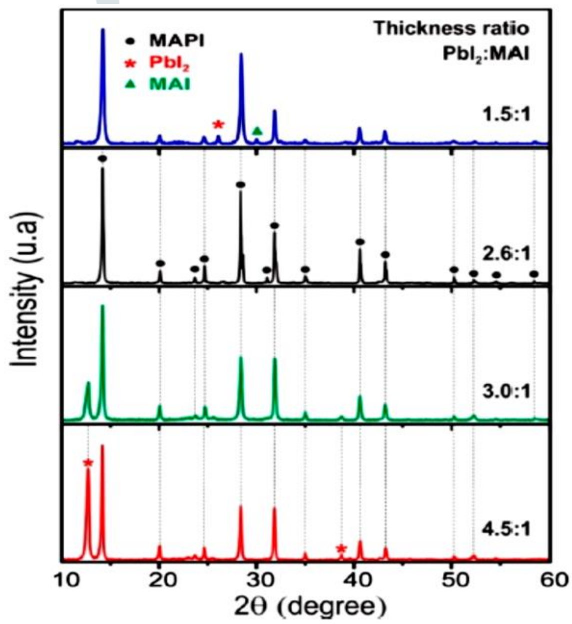

Figure 1. X-ray diffraction spectra of MAPI films prepared varying the lead iodide (PbI_2)/MAI

3.2 Morphological analysis

The influence of chemical composition on the morphology of MAPI film was studied through SEM measurements. Figure 2 shows SEM images corresponding to MAPI films prepared at room temperature varying the PbI_2/MAI thickness ratio. In particular, it is observed that the samples prepared with excess of MAI (1.5 to 1 ratio) present formation of large and elongated clusters surrounded by grains of nonmetric size. Taking into account the results of XRD that indicate that samples deposited with excess of MAI present formation of the MAI phase, we believe that the observed clusters could correspond mainly to the compound MAI. On the other hand, samples prepared with excess of PbI_2 (4.5 to 1 ratio) exhibit a porous morphology constituted by grains of sub-micron size of irregular shape. The SEM images also show that the MAPI samples prepared with chemical composition corresponding to a PbI_2/MAI thickness ratio of 2.6:1 exhibit a morphology consisting of compact grain structures with sub-micron size.

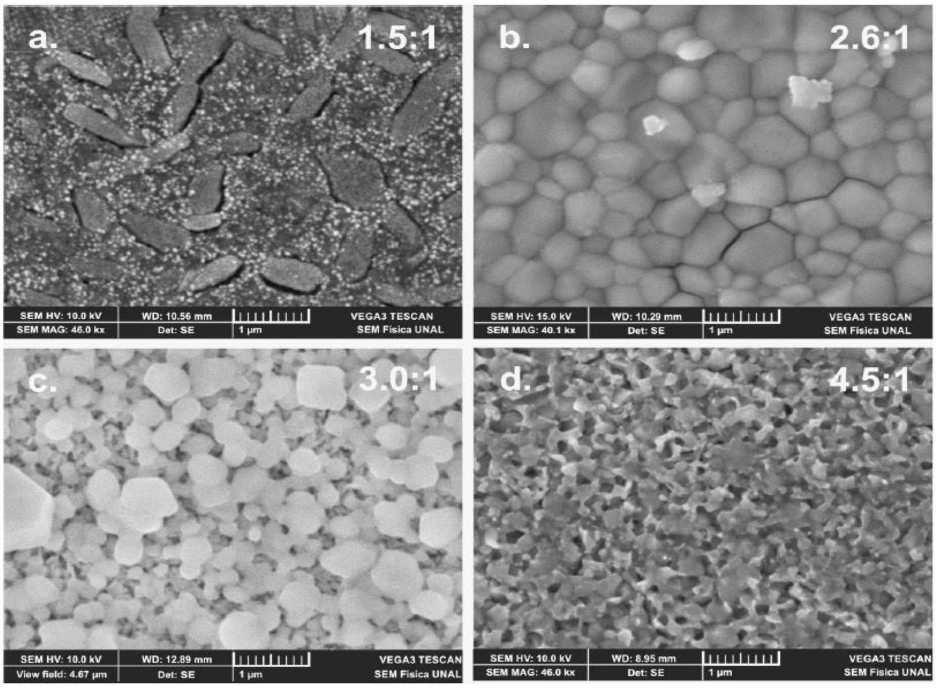

Figure 2. SEM images of MAPI films prepared at room temperature and PbI_2/MAI thickness ratio of (a) 1.5:1, (b) 2.6:1 (c) 3.0:1 and (d) 4.5:1.

3.3 Electrical Characteristics

Solar cells were constructed from the structure of Ag/CuI/MAPI /TiO_2 Nano films deposited on the substrate of FTO, and here MAPI film acts as an active layer in a photovoltaic material. In order to verify the reliability of the formation of the MAPI film to be work as an active layer during operating the device, we have to study the electrical Characterizations of this layer. The I-V curves measured under air mass (AM 1.5) light source 100 mW/cm^2 and active area 1cm2.To test the applicability of the MAPbI3 film developed in this work, a solar cell with an Ag/CuI/MAPI /TiO2 Nano films structure is coupled to an active layer in a photovoltaic device . Fig.3. shows the I-V curves of the solar cells that were fabricated using MAPI film as active layer.

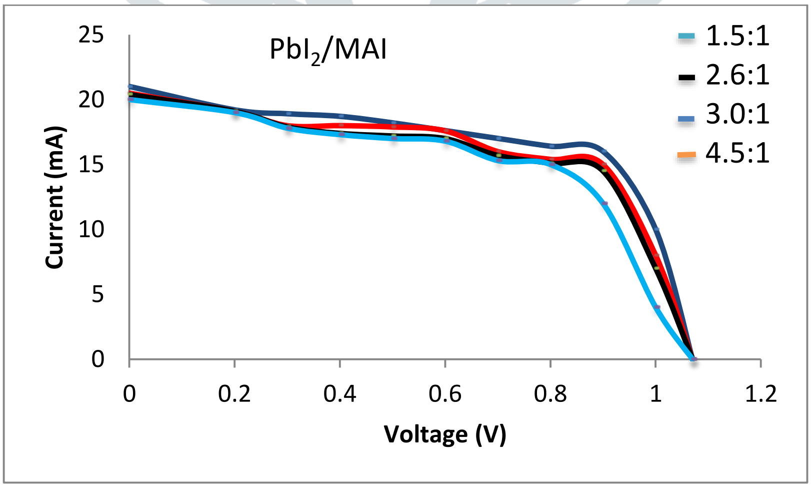

Fig.3. I-V curves of the perovskite solar cells prepared with structure Ag/CuI/MAPI /TiO_2 on FTO glass substrate with various thickness ratio (a) 1.5:1, (b) 2.6:1 (c) 3.0:1 and (d) 4.5:1.

Table (1) shows the values of the corresponding performance parameters (short circuit current J_{sc}, open circuit voltage V_{oc}, fill factor FF and efficiency η), And the influence of chemical composition of films on the performance parameter is also reported. These agree with values reported by other authors [18].

Table (1). Effect of chemical composition on cell performance (short circuit current (I_{sc}), open circuit voltage (V_{oc}), fill factor (FF) and efficiency)

Sample	Thickness ratio	I_{sc} (mA)	V_{oc}(V)	FF	η (%)
S_1	1.5:1	20	1.07	0.504	10.7
S_2	2.6:1	20.4	1.07	0.536	11.7
S_3	3.0:1	21.5	1.07	0.625	14.3
S_4	4.5:1	21	1.07	0.580	13

As can be seen from Fig.3. The main reason for the low efficiency is low FF and low short circuit current (J_{SC}), and part of the reason for low FF is the high series resistance of the device. The FF also depends on the quality indicator of the diode, which is affected by the reorganization of the trap centre in the degradation zone. Apparently, due to low charge transfer at the TiO_2/MAPI and CuI/MAPI interfaces. Due to the recombination of interface states, a high loss of photocurrent may be another factor that is a loss of short circuit current. The data reported in Table (1) shows that the annealing deposition of the PRK layer will meaningfully affect the short-circuit current, thereby affecting the device efficiency, the maximum short-circuit current and the efficiency acquired in the film prepared by thickness ratio 3.0:1.It has also been found that film manufactured using thickness ratio 3.0:1 under such conditions can achieve the highest efficiency, thereby reducing new phases, and exhibiting better morphology and better crystal structure.

IV. Conclusion

In summary, an appropriate thin film property has been manufactured by using two-step spin coating solution method of their precursors lead iodide synthesized from car battery and methylammonium iodide. The efficiency of our solar cells reached 14.3%. It was found that the CH3NH3PbI3 films synthesis or fabricated by using Pb from car battery and thickness ratio (PbI_2/MAI) 3.0:1 show good efficiency and high fill factor, and these films have higher efficiency than samples prepared at another molar ratio. Results of X-ray diffraction, indicated that the structure of films effected by chemical composition. The SEM results suggest that the thickness ratio treatment significantly changed the morphology of the MAPI film. It was found that the best thickness ratio of lead iodide/ methyl-ammonum iodide is (3.0:1).

REFERENCES

[1] National Renewable Energy Laboratory (NREL,2019). Best Research-Cell Eff. Available online: http://www.nrel.gov/pv/assets/images/effciency-chart.png
[2] Miyasaka T., Teshima K., Shirai U., Kojima A. (2009). Organometallic halide perovskite as sens. of vis light for PV cells. J. Am. Chemical Soc. 131, 6050-51.
[3] Noh, J.H ., Jeon, N. J., Yang, W.S ., Kim, Y. C., Ryu, S ., Seo, J ., Seko, S.I. (2015). Perovskite of Composal Eng Mat for high perf solar cells. Nature, 517, 476–480.
[4] Park, N.G. (2015). PSC: Emerging Photovoltaic Technology. Mater Today, 18, 65-72
[5] Green, M.A., Baillie, A.H., Snaith, H.J. (2014). The emergence of PSCs. Nat. Photonics 2014, 8, 506–514.
[6] Rangel-Cordenas, J., Sobral, H. (2017). absorption of optical enhancement in thin films CdTe by micro structuring a silicon substrate. Materials 10, 607.
[7] Shi, Z., Jayatissa, A.H. (2017). One-pot hydrothermal synthesis and fabrication of kesterite Cu2ZnSn(S,Se)4 thin films. Prog. Nat. Sci. Mater. Int., 27, 550–555.
[8] Kumar, M.H.; Yantara, N.; Dharani, S.; Graetzel, M.; Mhaisalkar, S.; Boix, P.P.; Mathews, N. (2013). Flexible, low-temperature, solution processed ZnO-based perovskite solid state solar cells. Chem. Commun., 49, 11089–11091.
[9] Liu, D.; Kelly, T.L. (2014). PSCs with a planar heterojunction structure prepared using room-temperature solution processing techniq. Nat. Photonics, 8, 133–138.
[10] Shin S.S., Yang, W.S., Noh, J.H., Suk, J.H., Jeon, N.J., Park, J.H., Kim, J.S., Seong, W.M., Seok, S.I. (2015). High-performance flexible PSCs using Zn2SnO4, prepared in solution below 100 °C. The Native Commun., 6, 7410.
[11] Hao, F., Stoumpos, C.C., Cao, D.H., Chang R.P.H., Kanatsidis, M.G. (2014). Lead-free solid-state organic-inorganic halide PSCs. The Native Photonics, 8, 489–494
[12] Zuo, C., Ding L. (2017). Lead-free perovskite materials (NH4)3Sb2IxBr9-x. Angew. Chemical, Int. Edition, 56, 6528–6532.
[13] Kawamura Y., Mashiyama H., Hasebe, K. (2002). Structural study of the cubic-tetragonal transition $CH_3NH_3PbI_3$. J. Phys. Soc. Jpn., 71, 1694–1697.
[14] Whitfield, P.S., Herron, N., Guise, W.E., Page, K., Cheng, Y.Q., Milas I., Crawford, M.K. Structures, phase transitions, and tricritical behavior of hybrid perovskite methylammonium lead iodide. Sci. Rep 2016, 6, 35685.
[15] Yousif, Kamil M & Abdulgafar, Sayran A. (2019). Low-cost solar selective absorbers by Electrodepositing technique. Publ. in book (Renewable Energy and Sustainable Buildings [ed.ProfA.Sayigh]. Springer International Publ. Switzerland 2019. chpt. 25, Selected Papers from the WREC 2018.
[16] Burschaka, N. Pellet, S. Moon et al. (2013). "Sequential deposition as a means of efficient perovskite-sensitized solar cells", Vol 1. 499, no. 7458, pages 316–319.
[17] Aziz, Issa M. (2020). Synthesizing and characterization of Lead Halide Perovskite Nanocrystals solar cells from reused car batteries. MSc. thesis, Dept of physics, Zakho University, Zakho, Iraq.
[18] Wang, Y., Liu, X., Zhou, Z., Ru, P., Chen, H., Yang, X., & Han, L. (2019). Reliable Measurement of Perovskite Solar Cells. Advanced Materials, 31(47), 1803231.