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Synthesis and Characterization of Methyl ammonium Lead Tri-Chloride: An active layer in Perovskite Solar Cell

KamalSolanki[1], ShilpaSharma[*], Pratibha Shrivastava[#]

[1]Assistant Professor, Rungta College of Engineering &Technology, Raipur, Chhattisgarh, India.

**Associate Professor, Rungta College of Engineering& Technology, Raipur, Chhattisgarh, India.*

[#] Professor, Rungta College of Engineering& Technology, Raipur, Chhattisgarh, India.

**Corresponding Author: Dr. Shilpa Sharma, Associate Professor, Rungta College of Engineering& Technology, Raipur, Chhattisgarh,*

Abstract

In this work, the preparation of $CH_3NH_3PbI_{3-x}Cl_x$ using Dimethylformamide as solvent by a Magnetic stirrer & hydrothermal method was done. The favorably smooth and dense surface morphology of the $CH_3NH_3PbI_{3-x}Cl_x$ layers are obtained & investigated in by UV- Visible spectroscopy. The results indicate that the $CH_3NH_3PbI_{3-x}Cl_x$ thin film possesses appropriate morphological, optical and electronic properties to be suitable for perovskite solar cell applications. The photovoltaic devices have been investigated and optimized in detail by tuning layer thickness, processing temperature and time, annealing conditions of interfacial layers.

Keywords: Perovskite Solar cell, Active layer, Magnetic stirrer, Hydrothermal synthesis

1. INTRODUCTION

A perovskite solar cell includes a perovskite structured compound, most commonly a hybrid organic-inorganic lead or tin halide-based material, as the light-harvesting

active layer. Perovskite materials such as methyl ammonium are cheap to buy and simple to manufacture, the rapid improvement of perovskite solar cells has made them the rising star of the photovoltaic's world and of huge interest to the academic community. Since their operational methods are still relatively new, there is great opportunity for further research into the basic physics and chemistry around perovskites. Furthermore, as has been shown over the past two years the engineering improvements of perovskite formulations and fabrication routine to significant increases in power conversion efficiency.

The perovskite lattice arrangement is demonstrated below. As with many structures in crystallography, it can be represented in multiple ways. The simplest way to think about a perovskite is as a large atomic or molecular cation (positively-charged) of type A in the centre of a cube. The corners of the cube are then occupied by atoms B (also positively-charged cations) and the faces of the cube are occupied by a smaller atom X with negative charge (anion).

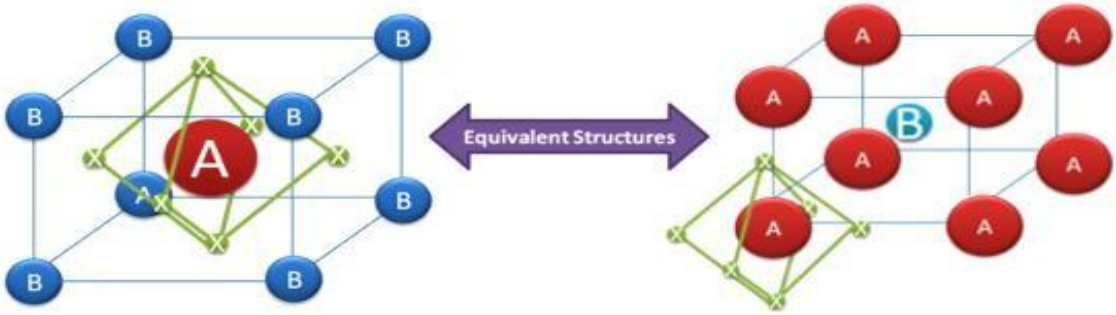


Figure no 1: Crystal structure of $CH_3NH_3PbX_3$ Perovskite (X=I,Br, andCl).

In the case of perovskite solar cells, the most efficient devices so far have been produced with the following combination of materials in the usual perovskite form ABX_3:

A=An organic cation-methylammonium$(CH_3NH_3)^+$

B =A big inorganiccation-usually lead (II) (Pb^+)

X_3=A slightly smaller halogenanion– usually chloride (Cl^-) or iodide(I^-)

Since this is a relatively general structure, these perovskite-based devices can also be given a number of different names, which can either refer to a more general class of materials or a specific combination. As an example of this, we've created the below table to highlight how many names can be formed from one basic structure.

A	B	X
ORGANO	METAL	TRI-HALIDE
METHYL AMMONIUM	LEAD	TRI IODIDE
	PLUMBATE	TRI-CHLORIDE

The perovskite name picking table**:** pick any one item from columns A, B or X3 come up with a valid name. Examples include: Organo-lead-chlorides, Methylammonium-metal-trihalides, organo-plumbate-iodides etc. The table demonstrates how vast the parameter space is for potential material/structure combinations, as there are many other atoms/molecules that could be substituted for each column. The choice of material combinations will be crucial for determining both the optical and electronic properties (e.g. band gap and corresponding absorption spectra, mobility, diffusion lengths, etc). A simple brute-force optimization by combinatorial screening in the lab is likely to be very inefficient at finding good perovskite structures. As such, while the field of perovskite solar cells has progressed rapidly so far with only a basic know-how of the photo physics and structural chemistry, far more in-depth knowledge than currently available is required to fully optimize devices.

2. EXPERIMENT:

2.1 Preparation of Methyl ammonium Iodide Crystal

0.3 mol (40 mL) hydroiodic acid (57 wt% in water, 99.95% pure, Sigma Aldrich) and equimolar methylamine (38 mL) (33 wt% in absolute ethanol, ≥99.0% pure, Sigma Aldrich) were mixed in 100mL ethanol with continuous stirring at 1200 rpm in an ice bath for 2h followed by evaporation at 60°C with continuous stirring at1200 rpm with the help of rotary evaporator until it completely forms white precipitate of CH_3NH_3I. The crystallite CH_3NH_3I was washed properly using diethyl ether $[(C_2H_5)O]$ (≥99.7%pure,with continuous stirring at 1200 rpm for 45 min and repeated same the step for five times and finally dried at 45 degree centigrade in an hot air oven for overnight.

2.2 Preparation of Perovskite Solution:

A) By Magnetic Stirrer Method:

The synthesis was based on the preparation of Perovskite solution with the treatment of magnetic stirrer. Firstly the Methyl ammonium iodide and Lead chloride were generally mixed in the Dimethyformamide to obtain the Perovskite solution by the molar ratio of (3:1)(Methyl ammonium iodide to Lead chloride),Then the total solution was ultrasonicated for around 30 minutes. At last, the thermal treatment 80 degree centigrade provided with the help of magnetic stirrer then we get yellow color.

B) Hydrothermal Method:

Firstly the Methyl ammonium iodide and Lead chloride were generally mixed in Dimethylformamide solvent to obtain perovskite solution by the molar ratio of (3:1) (Methyl ammonium iodide to Lead chloride). Then the solution was ultrasonicated for around 30 minutes, At last, it is heated at 80℃ with the help of Hydrothermal synthesis.

3. RESULT & DISCUSSION:

3.1 Optical property of Perovskite solution

The UV-VISIBLE measurement was carried on the Perovskite solution ($CH_3NH_3PbI_{3-x}Cl_x$), results by both the method were concluded, in case of magnetic stirrer method it was found that the λ_{max} is 390nm, and in case of Hydrothermal synthesis, found the diffraction peak at 380nm and 420nm, which indicates different shape & size of material (morphology difference) which is relatively good for Perovskite solar cell.

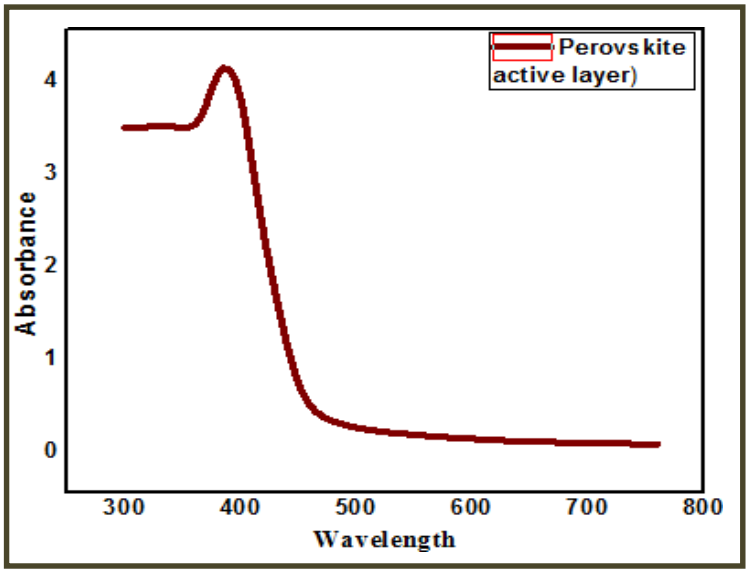


Figure 2: Absorption spectra of Active layer via Magnetic stirrer.

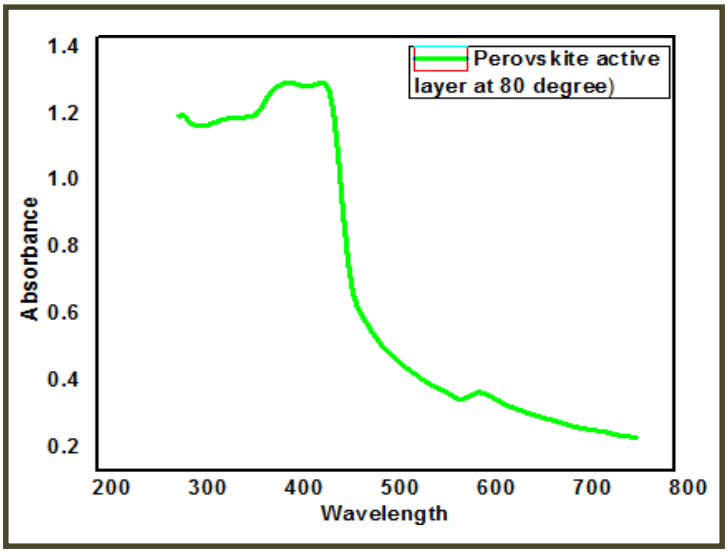
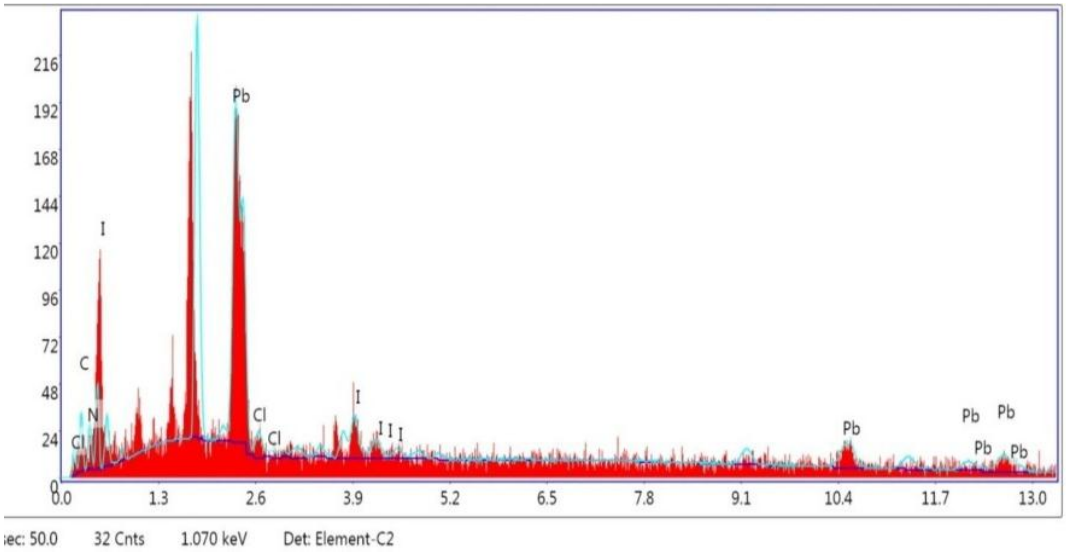


Figure 3: Absorption spectra of Active layer via Hydrothermal treatment.

3.2 Energy Dispersive X-ray spectroscopy:



ELEMENT	WT.%	ATOMIC WEIGHT%
CK	5.83	31.50
NK	8.36	38.71
PbM	71.28	22.32
ClK	0.02	0.04
IL	14.51	7.42

Figure. 4: EDX graph representing the various compounds present in the perovskite Solution with weight percentage also shown in figure.

3.3 Dual thermal annealing engineering technique

Fabrication of most-promising $CH_3NH_3PbI_{3-x}Cl_x$ based perovskite solar cell in ambient condition is excessively essential to industrialize this revolutionary development. In this research work, an efficient, facile and economical technique has been developed to fabricate $CH_3NH_3PbI_{3-x}Cl_x$ perovskite solar cell in ambient condition which is termed as dual-step thermal engineering technique .In this dual-step thermal engineering technique, the perovskite precursor solution has been spin coated over a mildly hot substrate which was heated at 60℃ for 10 min followed by

annealing at 80℃ for 30 min immediately after spin Coating.

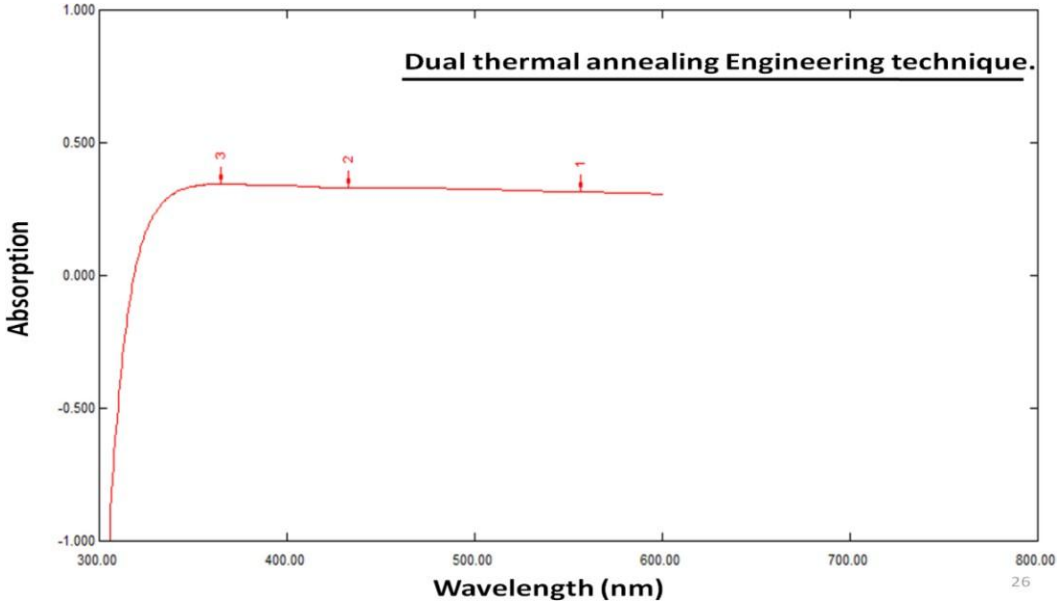


Figure 5: Absorption spectra of $CH_3NH_3PbI_{3-x}Cl_x$ Perovskite Film

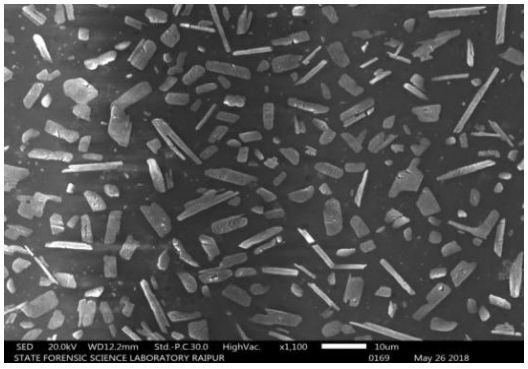


Figure 6: SEM morphology image of $CH_3NH_3PbI_{3-x}Cl_x$.

CONCLUSION

The Perovskite solution using Methyl ammonium iodide, Lead chloride & dimethyl formamide is synthesized by using magnetic stirrer & hydrothermal process. The characterization of the prepared perovskite solution was done from spectroscopic measurement. It is found that enhanced absorption Spectrum of $CH_3NH_3PbI_{3-x}Cl_x$ via hydrothermal synthesis are obtained at 80℃ with good optical properties & it was also found that two diffraction peaks were obtained at 380 nm & 400 nm because of heating effects which indicates difference in morphology & its relatively good for Perovskite solar cell which will enhanced absorption spectra of Perovskie layer & it

also enhance the power conversion efficiency of Perovskite solar cell. Overall, the simple & stable perovskite solution that is developed is a viable candidate of active layer in Perovksite solar cell.

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