Study of Interface Layer and Fabrication of Perovskite Solar Cell (PSC)

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Abstract: Perovskite solar cells (PSC) based on organometal halide light absorbers are considered as a promising photovoltaic technology due to their high power conversion efficiency (PCE) along with very low material cost. Since the first report on a long-term durable solid-state perovskite solar cell with a PCE of 9.7% in 2012, PCE as high as 19.3% was demonstrated in 2014, and a certified PCE of 17.9% was shown in 2014. In the present study, Perovskite Solar cells of the structure **ITO/PEDOT: PSS/$CH_3NH_3PbI_3$/LiF/Al** (Inverted structure) has been investigated. Fabrication of such cells involve cleaning the substrate, spin coating and deposition of the material on the substrate through thermal evaporation technique. After fabrication of solar cells, J-V characterization of these cells were carried out to determine the device parameters such as PCE, open circuit voltage (V_{oc}), fill factor (FF), and short circuit current density (J_{sc}). Future prospects of Perovskite Solar Cells are discussed.

Keywords: Perovskite Solar Cells (PSC), Organometal halides, Power Conversion Efficiency (PCE)

1. INTRODUCTION:

There is a current global need for clean and renewable energy sources. Fossil fuels are non-renewable and require finite resources, which are dwindling because of high cost and environmentally damaging retrieval techniques. So, there is an urgent need for cheap and sustainable resources. An efficient and more feasible alternative option is solar energy. Solar energy is more practical due to its plentiful availability; it is derived directly from the sun. Solar power is the key to a clean energy future.

PSC is a third generation solar cell. It consists of a perovskite compound, most commonly a hybrid organic-inorganic lead or tin halide based material, as the light-absorbing active layer. Perovskites possess intrinsic properties like broad absorption spectrum, fast charge separation, long transport distance of electrons and holes, long carrier separation life time that make them very promising materials for solid-state solar cells. Solar cell efficiencies of device using these materials have increased from 3.8% in 2009 to 22.1% in late 2017. PSCs are the fastest-advancing solar technology to date [1, 2, 3]. The structure of PSC is shown in Fig. 1. There are basically two types of PSC structures, one normal and the inverted. In the normal structure the electron transport layer (ETL) is sandwiched between the active perovskite layer and the Indium Tin Oxide (ITO) or Fluorine doped Tin Oxide (FTO) layer.

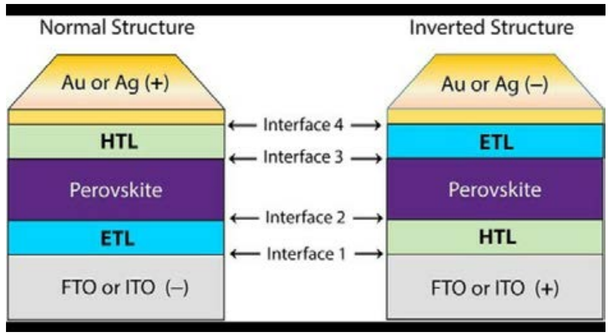

Fig. 1 Structure of Perovskite solar cell, ETL: electron transport layer. HTL: hole transport layer

where as the hole transport layer (HTL) is sandwiched between the perovskite layer and the metal (Au, Ag or Al) electrode. In the inverted structure the ETL and HTL layer positions are interchanged.

2. MATERIALS AND METHODS:

2.1 Materials

ITO: Indium Tin oxide (ITO) is colorless and transparent in thin layers, but it is yellow in bulk. ITO is a highly doped n-type semiconductor; it's band gap is around 4eV. In the present work ITO coated glass was used as one transparent electrode. It acted as the active layer to absorb light to generate free charge carriers. Its resistance was around 300-500 ohm/cm.

PEDOT:PSS (Hole Transport Layer-HTL): Poly (3,4-ethylenedioxythiophene) polystyrene sulfonate (PSS) is a polymer mixture of two ionomers. One component in this mixture is made up of sodium polystyrene sulfonate. Part of the sulfonyl groups are deprotonated and carry a negative charge. The other component PEDOT is a conjugated polymer and carries positive charges and is based on polythiophene. PEDOT:PSS is used as an antistatic agent to prevent electrostatic discharges during production and normal film use, independent of humidity conditions, and as electrolyte in polymer electrolytic capacitors.

PEDOT:PSS possesses many unique properties, such as good film forming ability by versatile fabricatipon techniques, superior transparency in visible light range, high electrical conductivity, intrinsically high work function and good physical and chemical stability in air. It has wide application in energy conversion and storage devices. PEDOT:PSS is being commonly used as the HTL.The mobility of hole in HTL is high.

The function of HTL is to transport the holes to the anode which are formed in active layer.When it is deposited above the ITO substrate, it avoid direct contact to the electrode with the perovskite layer and therefore increases the selectivity of the contact. This reduces the recombination of the holes and electrons(which are formed in the active layer) because it has high charge transporting properties as compared the active materials.

Methyl Ammonium Lead Iodide ($CH_3NH_3PbI_3$) (Active layer): $MAPbI_3$ plays an important role as a light absorber and long range hole diffusion length, at least 100 nm. It has either cubic or tetragonal lattice structure at room temperature. The bandgap of $MAPbI_3$ is 1.55eV. In the visible range the absorption coefficient of $MAPbI_3$ is around 1.0 x 10^5 (mol $L^{-1})^{-1}cm^{-1}$ at 550 nm. When the thickness of perovskite film ranges from 500-600 nm, it can absorb complete light in films (i.e no reflection of light will take place). At room temperature, $MAPbI_3$ crystallizes in a tetragonal unit cell. Above 327.4K, the unit cell undergoes a change in symmetry to become cubic, whereas below 162.2 K, the unit cell is orthorhombic. With a bandgap of 1.55 eV, this material is able to absorb incident light throughout the visible region and up to 800 nm. The valence and conduction band of $MAPbI_3$ are formed exclusively from Pb and I orbitals.

The methylammonium cation does not participate electronically in the band structure but governs the formation of the 3D perovskite crystal and therefore influences the optical properties of the material.

LiF (Electron Transport Layer-ETL): LiF has a good band alignment with adjacent layers and a good stability with the cathode interface. It stands out as a promising candidate due to its fabrication simplicity and stability. LiF is a wide band gap (>10 eV) material and is normally deposited via thermal evaporation. It is used as ETL to transport the electrons to the Cathode. It reduces the recombination of the free charge carrier with their counterparts which exist at the interface. It has high electron affinity and high electron mobility.

Aluminium: It is used as electrode. It is used to increase the work function of the ETL layer.

2.2 Experimental Procedure:

2.2.1 Active layer preparation

To synthesize the active layer CH_3NH_3 and PbI_2 were taken in desired concentration to prepare the perovskite absorber ($CH_3NH_3PbI_3$). Here 1:1 ratio of CH_3NH_3I and PbI_2 are used in DMF (Di methyl formamide) solution. The mixture was stirred for 12 hours with a magnetic bead at 70^0C.

2.2.2 Fabrication of Inverted PSC-Cleaning of the ITO substrates

Cleaning of the ITO substrate is an important step in the solar cell fabrication, because even a single particle or stain can disturb the uniformity of the film. Firstly the ITO coated substrate was washed with soap solution and DI (Deionized water) water. Then the substrate was sonicated for 15 minutes to remove the dust. In the next step, the substrate was rubbed by soap solution using cotton multiple times. After that sonication process was applied for 15 minutes. It was done to prevent ionic combination that may affect the proper operation of ITO. Then the substrate was boiled in acetone for 15-20 minutes in order to remove all the water droplets from the substrate. Finally, the samples were made to boil in Isopropanol for 20 minutes. It dissolved a wide range of non-polar compounds and acetone. It displaced water as well allowing surfaces to dry without spotting. Acetone leaves a residue, once dried is hard to remove, thus it was rinsed with isopropanol to remove the residue. Finally the substrate was put in vacuum oven at 100^0C for drying.

UV Ozone treatement

The UV-Ozone cleaning procedure is a highly effective method to remove a variety of contaminants from surfaces. This process has been carried out inside the glove box. A glovebox is a sealed container that is designed to allow one to manipulate objects when a separate atmosphere is desired

Coating of HTL layer and annealing

PEDOT:PSS was used as a hole transport layer. Coating of this HTL was done by a spin coater. The ITO substrate was kept inside the spin coater, held in high vacuum. The substrate was placed with ITO side facing up. Then the rpm was set for desired time. Spin coating is a procedure used to deposit uniform thin films on flat substrates. After that the substrates was annealed for 15 minutes at 140^0C for the evaporation of the solvent and to harden the deposited film into a semisolid form.

Coating of Active layer

Methyl ammonium lead iodide ($CH_3NH_3PbI_3$) was used as a active layer. The active layer was coated by spin coater at 1000 rpm for 30 sec and 3000 rpm for 30 sec for creating a uniform film. Thus the thickness of active layer was obtained was as 200nm. After this process, the substrate was annealed at 110^0C for 20-30 minutes.

Deposition of ETL layer

LiF was used as the ETL layer for PSC fabrication. Deposition of LiF layer was done using a thermal evaporator system. For this first a tungsten boat was flushed in which the material was to be loaded. The melting point of tungsten is 3422^0C. By resistive heating method the boat was flushed. Low vacuum of 3 X 10^{-2} Pa was created by a rotary vane pump and high vacuum of 5 X 10^{-6} Pa by a turbo pump. After that the LiF was deposited and then Al was deposited in the high vacuum atmosphere.

3. RESULT:

Current vs Voltage (J-V) curve of the inverted perovskite solar cell is shown in Fig. 2. Device parameters of fabricated perovskite solar cells are presented in Table 1.

Table 1: device parameters of fabricated perovskite solar cell

S.no	Device	Voc(V)	J_{SC}(mA/cm^2)	FF	Efficiency
1	ITO/PEDOT:PSS/MAPbI$_3$/LiF/Al	0.761	5.65X10^{-3}	0.202	0.8%

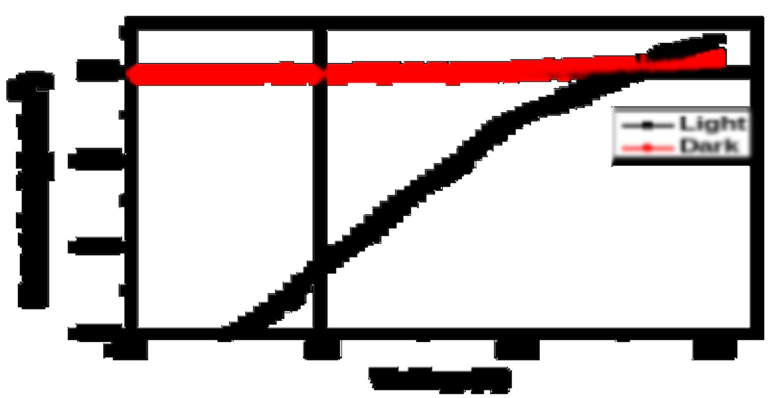

Fig.2 J-V Curve of the inverted perovskite solar cell

The efficieny of inverted device structure (ITO/PEDOT: PSS/$CH_3NH_3PbI_3$/LiF/Al) was expected to be 15%, but we got only 0.8%. The reasons of low stability are as follows-

- Degradation of perovskite material due to air
- Thickness and morphological issues in perovskite absorber and interfacial layer materials
- Ununiformity of Al electrode

CHALLENGE:- The long term stability of perovskite solar cells in a big issue. The degradation mechanism of perovskite materials is not clearly understood. An understanding of the degradation mechanism will be helpful to enhance the long-term stability, which will be a significant criterion for the commercialization of perovskite solar cells.

Water interacts strongly with commonly used perovskite material for solar cells,such as $MAPbI_{3.}$ As the structure is soluble in water, the presence of humidity during film processing can significantly influence the thin film morphology.

4. CONCLUSIONS:

Fabrication of the perovskite solar cells using inverted device structure **ITO/PEDOT: PSS/$CH_3NH_3PbI_3$/LiF/Al** was demonstrated and the efficiency of .80% was achieved. The recent progress made in the device architectures and new materials open new opportunities for highly efficient and stable perovskite solar cells.

5. FUTURE PROSPECTS:

The development of perovskite solar cells in the last few years makes it a promising alternative for the next-generation, lowcost, and high-efficiency solar cell technology. Driven by the urgent need of cost-effective, high-efficient solar cells, PSCs have been intensively investigated in the recent years. Undoubtedly, halide perovskite materials have emerged as an attractive alternative to conventional silicon solar cells. It is suitable for flexible solar cell due to the low temperature processing and high efficiency.

PSC can be applied in photo-electrodes, radiation sensing and many more fields. The major problems in commercialization of PSC is the presence of toxic lead.

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