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$Cs_3Sb_2I_9$- All inorganic lead free perovskite like material for solar cell application

Anupriya Singh[1,2,3], Karunakara Moorthy Boopathi[2], Chih Wei Chu[3]

[1]*Department of Physics, National Taiwan University No. 1, Sec. 4, Roosevelt Road, Taipei 106, Taiwan*
[2]*Research Center for Applied Science, Academia Sinica,128 Academia Road, Section 2, Nangang Taipei 115-29 Taiwan (R.O.C.).*
[3]*Nano Science and Technology Program Taiwan International Graduate Program Academia Sinica and National Taiwan University Taiwan*
Phone- +886-2-27873183, Email- gchu@gate.sinica.edu.tw

Abstract

All inorganic antimony based perovskite '$Cs_3Sb_2I_9$' has been investigated for photovoltaic performance. $Cs_3Sb_2I_9$ exists in two polymorphs and both showed photovoltaic (PV) performance. A comparison between photovoltaic properties showed layer polymorph (PCE = 1.02%) better than dimer polymorph (PCE= 0.62%) for PV applications.

1. Introduction

Replacement of lead (Pb) to other element which can have similar valence shells like Pb can remove the obstacle of toxicity in Pb based perovskite solar cells, while low stability can be dealt by replacing moisture and temperature sensitive organic cations by inorganic cations like Cesium (Cs).[1] Antimony based perovskite like structures are recently emerging for photovoltaic applications. Highest reported is 0.66 % for $Rb_3Sb_2I_9$.[2] All inorganic $Cs_3Sb_2I_9$ occurs in two types of polymorphs, first has two dimensional corrugated layers of polyanions and second has isolated bi-octahedral $Sb_2X_3^{9-}$ anion.[3] Theoretical studies have postulated layer to be a better material for photovoltaic (PV) applications because of its nearly direct band gap, higher electron and hole mobilities and better tolerance to defects because of higher dielectric constants than the dimer form.[2] Usually solution processing favors dimer form but by sequential introducing SbI_3, we prepared layer from by solution process.[4] Also, the DFT calculations showed that the material has deep level defects which limit its open circuit voltage (Voc) below 0.2 V and current density (Jsc) below 0.2 mA/cm^2.[2] Here, we studied the films formed for both the polymorphs by solution processing method. The formation of polymorphs was confirmed by XRD pattern. A PCE of 1.02 % has been achieved by using layer form as active layer while dimer form also showed PV performance with PCE to be 0.62 %.

2. Results and discussions

A single precursor solution was prepared by mixing 0.25M of SbI_3 and 1M of CsI in DMSO:DMF (0.75:0.25) mixture was dropped on the PEDOT:PSS coated substrates and spin coated for 40s at 6000rpm. For preparation of dimer form, films were annealed at 150 ^oC while for layer $Cs_3Sb_2I_9$ films (2 samples at a time) were annealed at 70^0C for 15 min and then directly moved to 250^0C in glass bottle (diameter 3cm X height 6cm). Then, this bottle is covered with cap after adding 30 µl (30wt%) of SbI_3 in DMF in the corners of bottle. The crystallinity of thin films corresponding to both the polymorphs was studied by X-Ray diffraction (XRD) method as shown in fig. 1(a). The strongest peak in simulated XRD spectrum of $Cs_3Sb_2I_9$ is at 2θ value of 25.7^0 corresponding to the (201) plane.[4] High intensity of peaks for layer polymorph in comparison to dimer was observed, showing the higher crystallinity in sample corresponding to layer polymorph. Besides the presence of the signature peak of $Cs_3Sb_2I_9$ at 25.7^0 i.e. for (201) plane, peaks at 8.67^0, 17.24^0 and 25.86^0 corresponding to (001), (002) and (003) respectively, shows the preferred C-axis orientation in the film. Full width at half maximum (FWHM) of the peaks was used to find the crystallite size.[5] The crystallite sizes of the layer and dimer $Cs_3Sb_2I_9$ were calculated to be 218 nm and 50 nm, respectively. So, the crystallinity and crystallite size of the layered perovskite film were found to be significantly higher than dimer form.

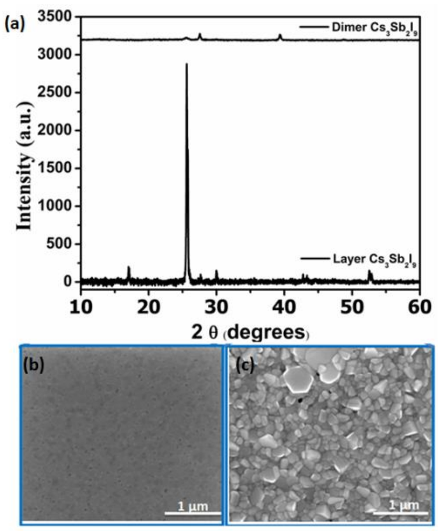

Fig. 1 XRD patterns of both the polymorphs showing their crystallinity; (b) SEM photograph for dimer; (c) SEM photograph for layer polymorph.

Morphology of the samples was studied by Scanning electron microscope (SEM). The crystallite size of about 200 nm can be seen in SEM of layer film (fig. 1b) while films corresponding to dimer form (fig. 1c) were found to be very smooth. Both the films were found to be uniform with very less pinholes.

The Planar Heterojunction (PHJ) solar cells were fabricated using both dimer and layered $Cs_3Sb_2I_9$ thin film as light absorber to explore their photovoltaic performance. Devices were made with the architecture (ITO/PEDOT:PSS/$Cs_3Sb_2I_9$/$PC_{70}BM$/C_{60}/BCP/Al). Fig. 2 shows photocurrent density-voltage (J-V) curve of the best devices obtained for dimer and layered form. The photovoltaic parameters are selectively summarized in Table 1. The champion device based on the lead-free inorganic layered $Cs_3Sb_2I_9$ perovskite showed J_{sc} of 3.84mAcm^{-2}, an V_{oc} of 0.63V with fill factor (FF) of 41.36% under AM1.5G solar illumination, corresponding to a PCE of 1.02% while the champion device corresponding to dimer form gave Jsc of 2.31 mAcm^{-2}, V_{oc} of 0.56V with FF of 47.32% for a PCE of 0.62%.

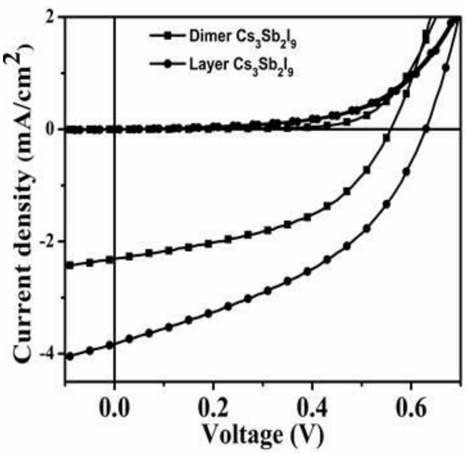

Fig. 2 Comparison of J-V characteristics of layer and dimer form

Table I Device performance of both dimer and layer form of $Cs_3Sb_2I_9$

$Cs_3Sb_2I_9$	Jsc(mA/cm^2)	Voc (V)	PCE (%)	FF (%)
Dimer	2.31	0.56	0.62	47.32
Layer	3.84	0.63	1.02	41.36

3. Conclusions

Based on the results presented here, we conclude that the layer $Cs_3Sb_2I_9$ perovskite has very promising properties for use in optoelectronic devices and solar cell performance of dimer is also appreciable and can be studied further.

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