Inorganic cesium lead mixed halide based perovskite solar materials

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Abstract

Herein, we examine the impact of cesium on the structural, morphological, optical properties and degradation of perovskite $CsPbBr_3$. Its structure, surface morphology and optical properties have been investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM) and UV-Visible spectrometer. The structure of perovskite thin films was found to be in the direction of (110) plane. It is seen from the XRD results that this kind of cation assumes a significant part in stabilizing and improving the performance of $CsPbBr_3$ based solar cells. Here, the cesium lead iodide thin films show a smooth and homogenous surface and enormous grain size without pinhole perovskite film. An optical investigation uncovered that the band gap is in a range from 1.4 to 1.8 eV for the different cations. Additionally, in ~60% humidity under dark conditions for two weeks, the structural and optical properties of $CsPbBr_3$ films remained good.

Introduction

Perovskite solar cells have been attracting attention for more than 10 years, with only 15 years of existence. The best known are $MaPbX_3$, because its yield has exceeded silicon photovoltaic technologies. However, the organic Methylamonium (Ma) part is the weak point of this perovskite, given its low lifespan. This is also the case for $FaPbX_3$-based perovskites, although Formamidinium is more moisture resistant with better stability, it is also an organic compound with a low duration. As a result, more and more research is directed towards inorganic compounds, especially Cesium-based, which are much more stable. [1,2]As part of this work, we study the $CsPbBr_3$ binder.

Various approaches have been explored to synthesized $CsPbBr_3$ by a variety of techniques such as spin coating, spray deposition, atomic layer deposition and chemical bath deposition.

Among all these techniques spin coating used to synthesize $CsPbBr_3$, due to inherent advantages such as simplicity, trouble-free, inexpensive and time-efficient. The synthesized $CsPbBr_3$ has characterized X-ray diffraction, surface morphologies, chemical composition, topography, Optical absorption and photoluminescence response.

Experimental Details

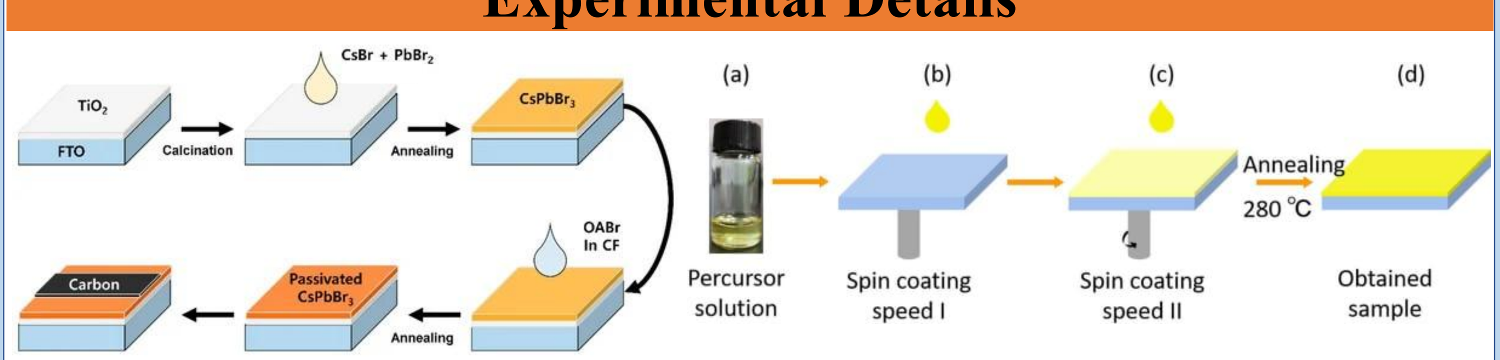

Fig 1 Manufacture of perovskite solar cells

Attributed to its high stability and wide band gap, CsPbBr3 perovskite has huge potential applications especially in semi-transparent and tandem solar cells. However, its low efficiency of $CsPbBr_3$ CSP hinders its commercialization due to the low crystallinity of the absorbent layer. Therefore, in this work, we use a dopant, Ytterbium (Yb) as a dopant. We prepared 5 solutions of perovskite $CsPbBr_3$, with concentrations of 0,1,2,4 and 8% Yb, with the technique of spin coating.

Resultes and Discussion

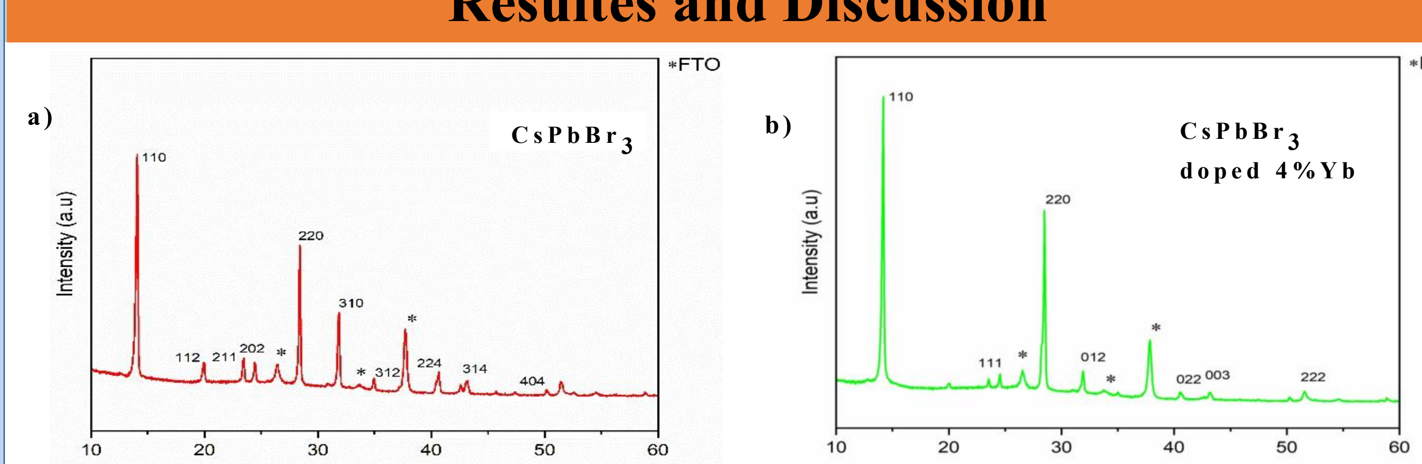

Fig 2. XRD of $CsPbBr_3$.

- The thin films $CsPbBr_3$ and $CsPbBr_3$ doped 4% Yb were examined by XRD in **Fig. 1(a)**, it is observed from the XRD analysis that several diffractions peaks are located at 14.0, 24.0, 28.0, 32.0, 37.5 and 52.0, which corresponds to the planes of (110), (202), (220), (222), (400) and (303) respectively.

- The FWHM and crystallite size was calculated from the XRD analysis by using Scherrer formula.

Table 1: The grain size, dislocation density and lattice strain of XRD of $CsPbBr_3$ and $CsPbBr_3$ doped 4% Yb thin fil diffraction peaks are correlated the previous $CsPbBr_3$ structure study [9,10]. In addition, the replace Pb by 4% Yb it was found that the intensity of the peak (110) increased. All perovskite films crystallize in a tetragonal lattice corresponding to the space group I4/mcm. The lattice parameters were found to be a = b = 8.919 Å, c = 11.920 Å

Sample.ID	Grain Size (nm)	Roughness (nm)	Dislocation density (nm^{-1})	Lattice strain (ε)
Pb	400	46.73	0.62×10^{-05}	0.39
Yb	300	36.99	1.11×10^{-05}	0.37

SEM, TEM and AFM analysis

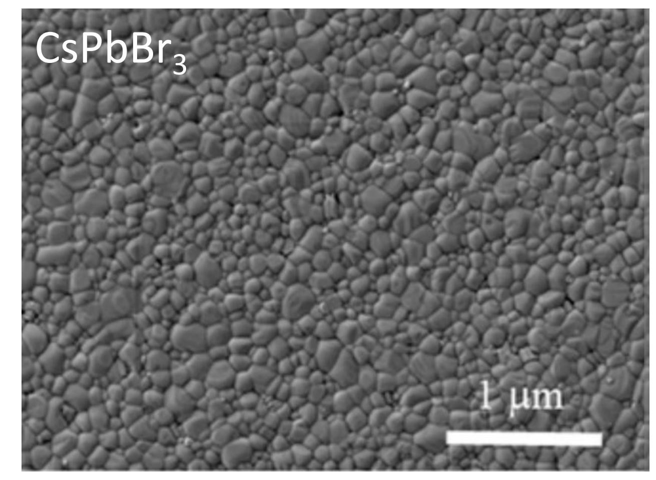

Fig 3. SEM análisis of $CsPbBr_3$ pure

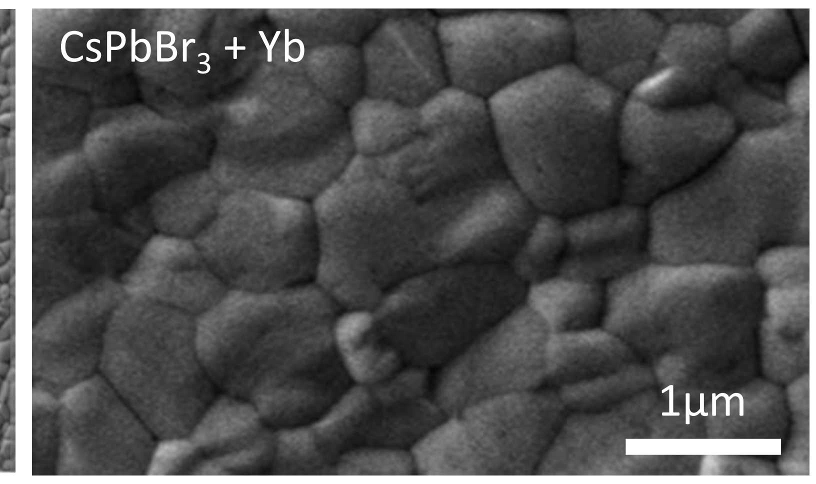

Fig 4. SEM analysis of $CsPbBr_3$ doped 4% Ytterbium

- Yb Replacement of Pb by Yb has a significant impact on the crystallization process of perovskite materials and produces an increase in the grain size of the perovskite thin film, as seen by SEM pictures,

Optical analysis

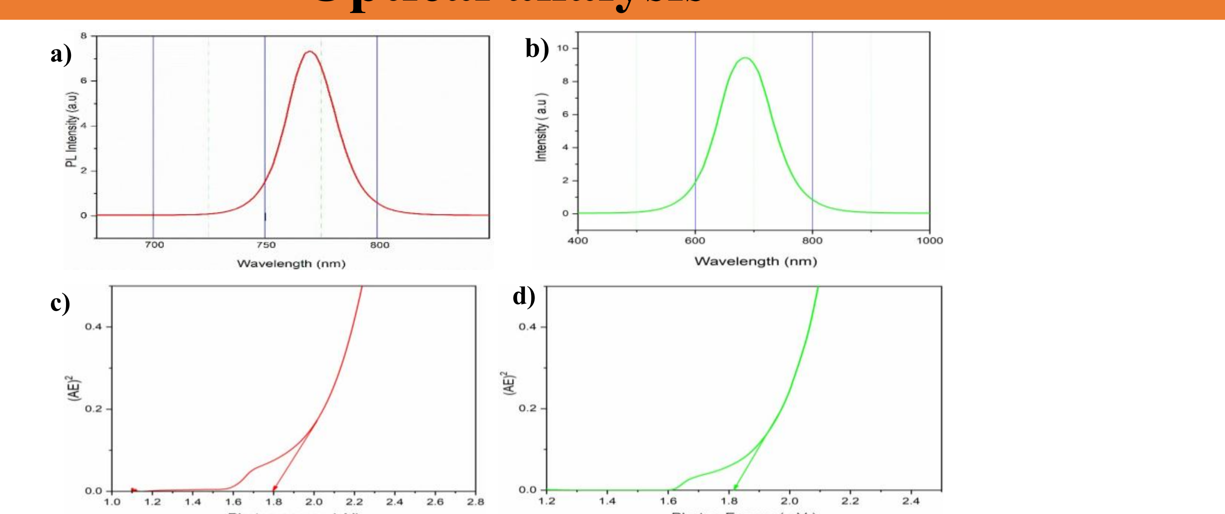

Fig 5. PL spectra a) $CsPbBr_3$ b) $CsPbBr_3$ doped 4% Yb **and** bandgap of c) CsPbBr3 d) CsPbBr3 doped 4% Yb

- UV-Vis in the range of 750 to 900 nm.
- Resultant bandgaps 1.82, 1.8 eV
- enhanced electron-hole pairs generation.
- PL measurement was recorded in the range of 500-1100 nm as represented in Figure 5. The PL peak intensity in the region of 700-900 nm is in good agreement with the previously reported study of $CsPbBr_3$. The measured intensity of the PL peak in $CsPbBr_3$ doped 4% Ytterbium films is about 30% higher than in $CsPbBr_3$ films

Degradation of $CsPbBr_3$

For evaluate the degradation of CsPbBr3, we examined samples fresh and 4 weeks aged in 60% of humidity under dark. By XRD patterns we have observed less intensity of peaks characteristics to CsPbBr3-Samples for aged sample and apparition of the new peaks characteristics of PbBr2 which give an idea about the rate of degradation. Further, we examined the surface of the layer by the SEM, the morphology of the perovskite layer CsPbBr3 showed a granular and rather inhomogeneous topography and grain boundaries which is ideal for the study of the degradation process. The degradation of CsPbBr3 doped 4% Yb prouved that Ytterbium stabilize the material. Our results can explain the rate of degradation and the origin of the enhanced performance and stability.

Conclusion

- The diffraction peaks show polycrystalline nature without any impurity peaks and the homogeneous morphology confirmed by SEM microscopy.
- The tunable bandgap was found in the range of 1.8 eV by replace a part of Pb.
- Optimizing the inclusion of Yb in perovskite can significantly enhance stability, according to our research.

Acknowledgements

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References.

1 Saad Ullah, Jiaming Wang, Peixin Yang, Linlin Liu, Shi-E. Yang, Tianyu Xia,, Haizhong Guo and Yongsheng Chen (2020). All-inorganic CsPbBr3 perovskite: a promising choice for photovoltaics. Materials advances 2, 646.

2 Chuanliang Chen, Xiaoman Lu, Xuzhi Hu, Guijie Liang and Guojia Fang (2024). Solution fabrication methods and optimization strategies of CsPbBr3 perovskite solar cells. The journal of materials chemistry C, 12, 16