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Shedding Light on Phase Stability and Surface Engineering of Formamidinium Lead Iodide ($FaPbI_3$) Thin Films for Solar Cells †

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Abstract: In this work, $FAPbI_3$ thin films with different antisolvents (toluene, diethyl ether and chlorobenzene) were successfully elaborated by the spin coating technique to study the influence of the different antisolvents in the films. The crystal structure, surface morphology and optical properties were characterized by X-ray diffraction (XRD), field-emission scanning electron microscopy (FESEM) photoluminescence and UV–visible spectrometry. According to XRD, the crystalline structure of $FAPbI_3$ was found in the orientation of the (110) plane, and it is observed that the type of antisolvent content in the absorber layer plays an important role in the growth and stabilization of the film. Here, chlorobenzene leads to a smooth and homogenous surface, a large grain size and a pinhole-free perovskite film. Additionally, the optical analysis revealed that the band gap is in the range from 1.55 to 1.57 eV. Furthermore, in an approximately 60% humidity environment and after two weeks, the stability and absorption of $FaPbI_3$ showed low degradation.

Keywords: $FaPbI_3$; perovskite; thin film; antisolvent

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1. Introduction

The logarithmic increase in the research and founding in the field of organic–inorganic halide perovskite (HOIP) thin films for solar cells represents a great opportunity for improving the efficiency and the stability of perovskite solar cells. HOPI have showed a power conversion efficiency of 25.5% [1] and optimal properties when used for solar cells. However, researchers are still facing the issues of commercialization of perovskite solar cell (PSC) devices, such as long-term stability.

In this work, we tried to study the influence of the antisolvent in the α-(FA)-based $FaPbI_3$ absorber layer of the PSC. According to previous research, the antisolvent plays a key role in the properties and the growth of the perovskite thin films [2].

2. Materials and Methods

2.1. Elaboration

The thin films were elaborated on FTO substrates of size 2.5 × 2.5 cm. The substrates were cleaned for 15 min in detergent, ethanol (LabKem), acetone (VWR Chemicals) and isopropanol (VWR Chemicals) in an ultrasonic bath. Afterwards, they were put in the UV-ozone for 15 min.

$FaPbI_3$ precursor solution was prepared by dissolving FaI (1M) and PbI_2 (1.05M) in DMSO and DMF solutions at room temperature. The solution prepared was left at 80 °C inside the glovebox for two hours, and afterwards it was filtered with a PTFE filter. Then, 50 µm of the solution was dropped onto the FTO substrate to elaborate the thin films using the one-step spin coating technique. Then, 1 mL of toluene, chlorobenzene or diethyl ether was dropped on the substrates while being statically spin coated at 2000 rpm for 10 s,

followed by 5000 rpm for 50 s. Afterwards, the samples were annealed for 10 min at 220 °C and stored in an inert Ar atmosphere.

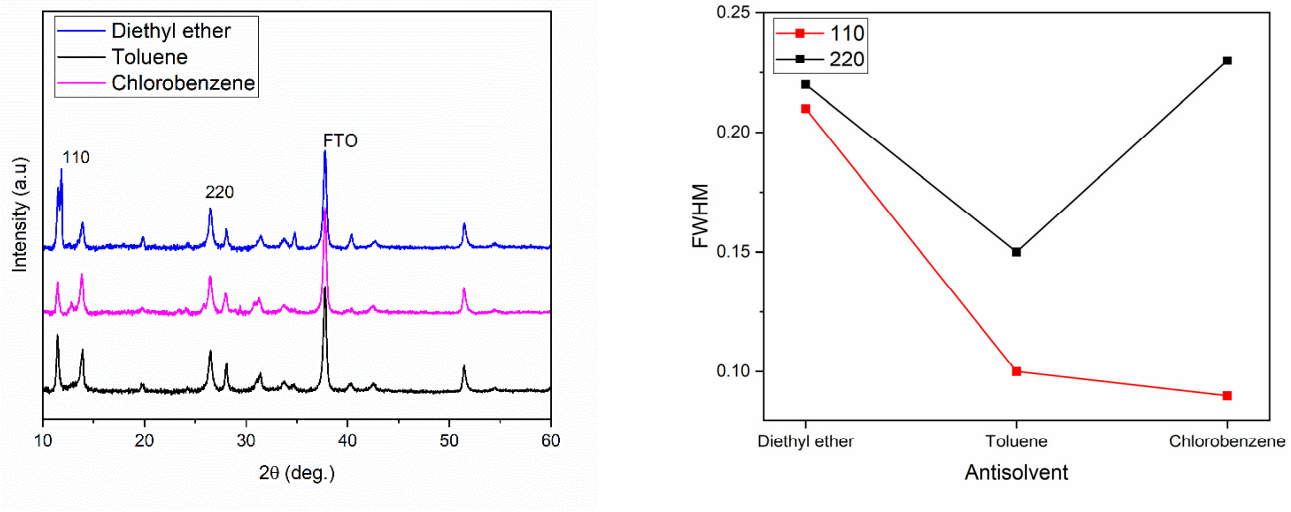
2.2. Characterization

The different thin films of $FaPbI_3$ elaborated with different antisolvents were first characterized by X-ray diffraction RIGAKU Ultima IV with Cu kα radiation (λ = 1.5418 Å). Afterwards, the optical properties were measured with Ocean Optics HR4000 spectrophotometer by a Si-CCD, and the photoluminescence (PL) emission source was a He-Cd laser at 405 nm. In the end, surface analysis of the samples was carried out by FESEM analysis.

3. Results and Discussion

3.1. XRD Analysis

The different α-$FaPbI_3$ films elaborated by spin-coating with different antisolvents were first scanned by X-ray diffraction analysis (XRD) (Figure 1a). The characteristic peaks of the perovskite (110) and (220) are located at 14.0° and at 28.1°, respectively. The peaks reported correspond to peaks reported previously [3]. From this analysis, we can say that the three samples show the growth of the material on the substrate.



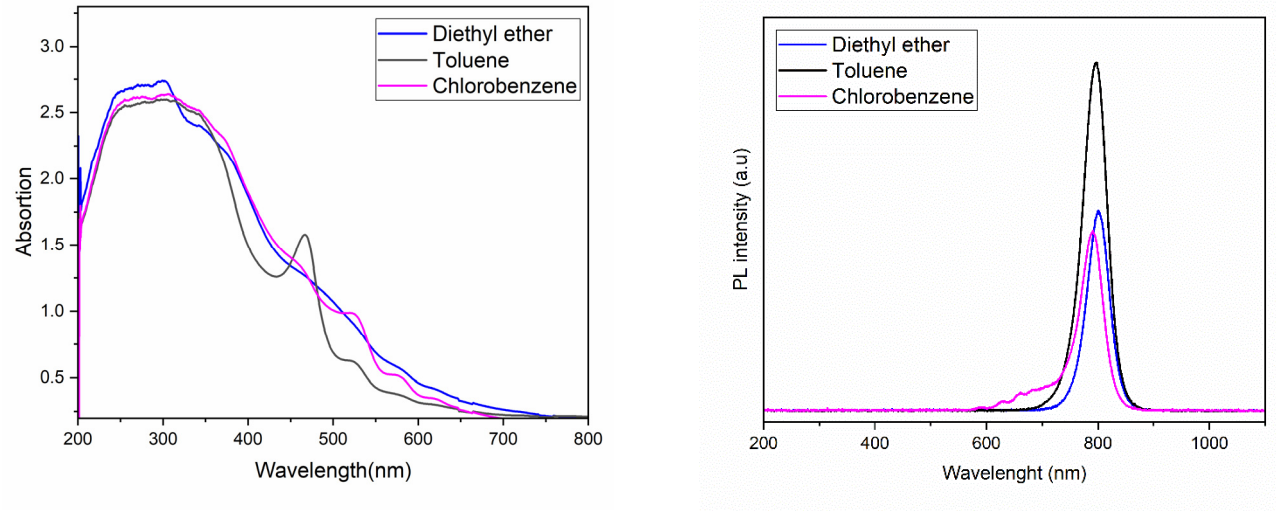
(**a**) (**b**)

Figure 1. (**a**) XRD patterns of $FaPbI_3$ with different antisolvents. (**b**) FWHM of characteristic peaks of $FaPbI_3$ with different antisolvents.

When calculating the full width half maximum (FWHM) (Figure 1b) of the two characteristic peaks, we report that toluene is the one that gives the sample better crystallinity, as it shows lower FWHM when compared to the other antisolvents.

3.2. Optical Properties

PL and absorption studies were performed to know the impact of the antisolvent in the optical properties of the devices. UV–visible absorption spectra of the different films were recorded between 200 and 800 nm (Figure 2a). The reported graph shows greater absorption when using diethyl ether as an antisolvent. The absorption tendence line is in good agreement with the literature [4]. However, from the PL analysis (Figure 2b), it is shown that the thin film elaborated with toluene as an antisolvent shows the greatest PL intensity. The PL intensity in the perovskite absorber layer is related to the viability of the material as a solar cell, as there is a correlation between the ability to emit light and the efficiency of a solar cell [5]. Additionally, the PL peak is located at 800 nm.



(**a**) (**b**)

Figure 2. (**a**) UV-visible absorption of $FaPbI_3$ with different antisolvents. (**b**) PL perovskite thin films of $FaPbI_3$ with different antisolvents.

Table 1 shows the calculated bandgap from the PL graph. The bandgap for the three different values is in the range of 1.55–1.57 eV, which corresponds to the optimal bandgap for α-$FaPbI_3$, as previously reported [6].

Table 1. Bandgap of $FaPbI_3$ thin films with different antisolvents.

Sample ID	Bandgap	
	λ (nm)	Eg (eV)
Diethyl ether	800.48	1.55
Toluene	795.55	1.56
Chlorobenzene	790.42	1.57

3.3. Surface Analysis

For surface analysis of the samples, FESEM analysis was performed. Figure 3 shows the top-view images of the films for the three antisolvents. All three images show a smooth surface. Nevertheless, the grain size is bigger in the toluene sample, and also, we see fewer small particles that complicate the definition of the grain edges in the FESEM images. This indicates that toluene may have a higher evaporation rate, which is important for the growth of the material in the films [7,8].

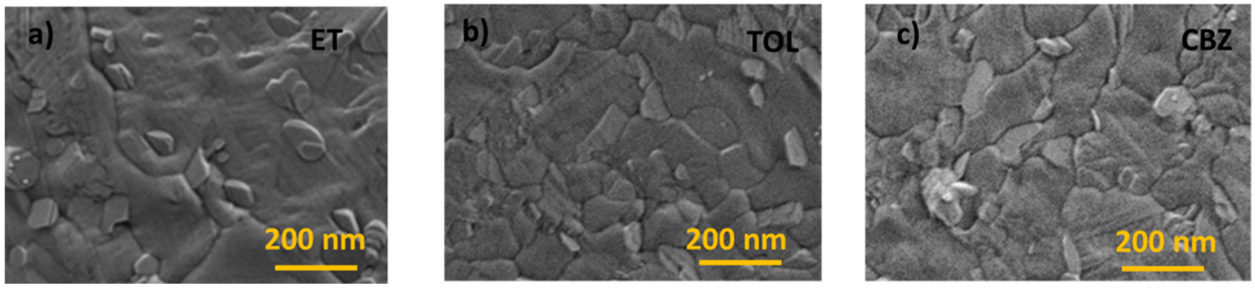


Figure 3. FESEM top-view images of $FaPbI_3$ thin films elaborated with different antisolvents; diethyl ether (ET), toluene (TOL) and chlorobenzene (CBZ).

4. Discussion

In this work, $FaPbI_3$ perovskite thin films were elaborated by the spin-coating technique using three different antisolvents to study the impact of the antisolvent on the optical properties and the surface morphology of the absorber layer of the PSC.

According to results reported above, toluene may be the best option for better performance of the cell as it shows greater crystallinity, higher PL intensity and greater grain size. This may be related to the evaporation effect the toluene has in the solvent (DMSO and DMF). We can confirm that for α- $FaPbI_3$ films, using DMSO and DMF as the solvent, toluene is the optimal antisolvent.

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