Review: Material characterization of an organic-inorganic hybrid for use in solar cells

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Abstract

Hybrid perovskite solar cells, which use low-cost deposition techniques, have made a lasting impression on the photovoltaic industry as a promising photo absorber material. The great efficiency and low cost of production of $CH_3NH_3PbI_3$ have made them very popular in solar applications. X-ray diffraction was used to determine $CH_3NH_3PbI_3$'s structural characteristics. The variability of the absorbance of $CH_3NH_3PbI_3$ across wavelengths of 300–800 nm is demonstrated by UV–visible spectroscopy. Under ambient processing conditions (about 50% relative humidity), we report the successful use of dibutylethanolamine (DBEA) as a multifunctional morphology-controlling ingredient to create high-quality homogenous films with grain sizes as big as ~5 μm. Compared to dimethyl sulfoxide (DMSO)-based perovskites, DBEA was able to produce a stable and homogeneous absorbing layer with a higher degree of efficiency because of its capacity to donate lone pairs and form hydrogen bonds with the inorganic octahedra of perovskite crystals.

Keywords: Perovskite solar cell, ambient air stability, High efficiency, Structural characteristic

1. Introduction

The sun is the source of all energy on Earth and has the capacity to produce clean, limitless energy. Solar cells are the most promising photovoltaic device to address these severe energy and environmental issues brought on by the usage of fossil fuels since they directly transform absorbed sunlight into power [1]. The commercial markets are now dominated by crystalline silicon (Si) solar cells due to their high power conversion efficiency (PCE) and greater stability. With a power conversion efficiency (PCE) of 25.2%, organic-inorganic hybrid perovskites have drawn a lot of attention as solar harvesters due to their excellent charge separation properties, tunable band gaps, broad absorption range, and high carrier mobility and absorption coefficient [2]. The most researched perovskite materials for solar cells in terms of simulations and manufacturing techniques are hybrid organic-inorganic halide compounds. Due to their low-cost production procedures, hybrid perovskites have been a "hot spot" for many solar cell researchers' research in recent years. [3] High conversion efficiencies have been demonstrated by solar cells that use a perovskite structure and the $CH_3NH_3PbI_3$ molecule. It has been demonstrated to be compatible with solar radiation, which qualifies it as a suitable material for solar-powered devices [4].

This paper reports on and discusses the characterization of perovskite materials for solar cells.

2. Results and discussion

2.1. Structural Properties

The perovskite films' X-ray diffraction patterns are shown in Fig. 1. According to plane (1 1 0), the peak at 14.06 degrees represents the orthorhombic crystal structure of perovskite [5]. The XRD pattern clearly shows the presence of an additional minor peak at 12.60, indicating that

a small peak of PbI_2 remained insoluble during the production of the absorber solution. The Scherer formula can be used to get the $CH_3NH_3PbI_3$ crystalline size from full width at half maximum (FWHM) as follows:

$$D = \frac{0.89\lambda}{\beta . cos\theta}$$

where the crystalline size of the crystal, the X-ray wavelength, the diffraction angle, and the full width at half maximum of the peak in the XRD pattern are represented by the parameters D, λ, θ, and β, respectively.

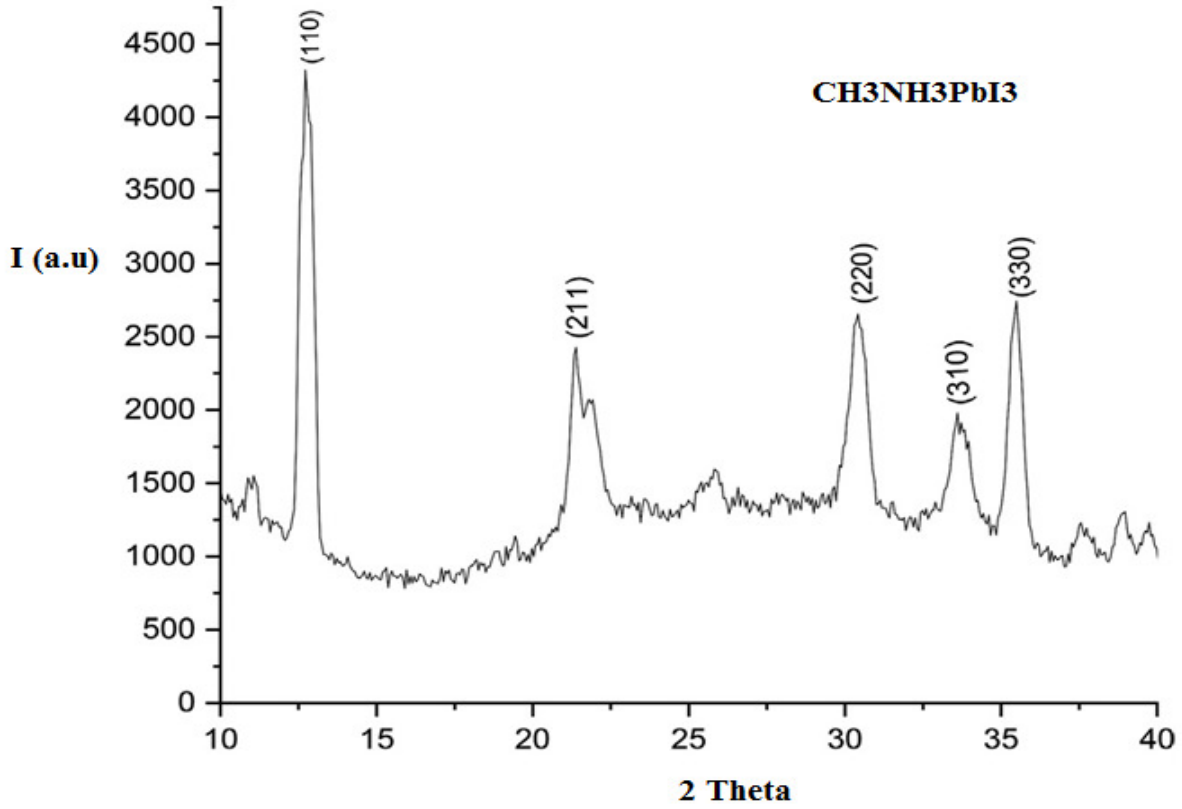

Fig. 1. X-ray diffraction (XRD) of $CH_3NH_3PbI_3$ perovskite

2.2 .Optical property of the perovskite film

The picture displays the $CH_3NH_3PbI_3$ perovskite material's optical absorbance spectrum. The change in absorbance as a function of the Wavelength between 300 and 800 nm for the

$MAPbI_3$ films is seen in Fig. 2, with two prominent and separate photo induced peaks, the spectrum is well confined, confirming the production of perovskite materials.

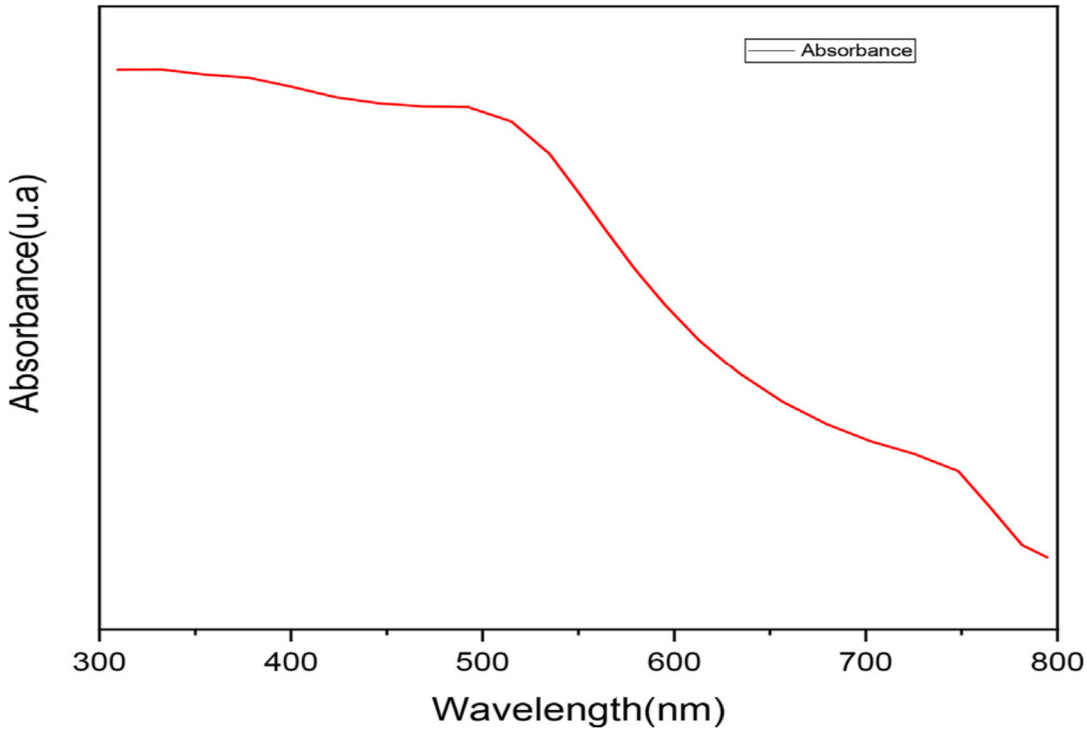

Fig. 2. Optical absorbance spectrum of $CH_3NH_3PbI_3$

Fig. 3 displays the perovskite films' X-ray diffraction profiles. The crystals generated using the DSPVD approach and the BC method essentially has identical XRD patterns. It is observed that the peak quantity varies somewhat. Furthermore, for the DSPVD sample, two additional peaks were detected at 12.95◦ and 29.96◦. These could be the reflections of PbI2 and MAI as a result of inadequate reactions during the deposition. The UV–Vis diffuse reflectance spectra of the

$MAPbI_3$ perovskite films are displayed in Fig. 4. Strong light absorption is shown by the perovskite layer up to around 790 nm, which is in line with reports in the literature [6].

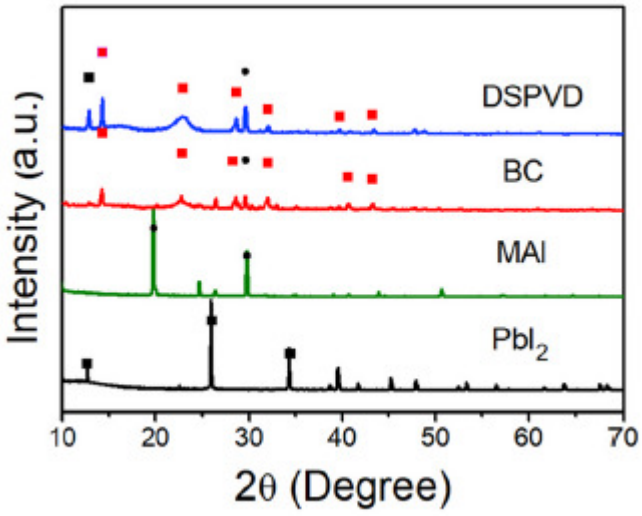

Fig.3. Shows XRD patterns of $MAPbI_3$ perovskite films.

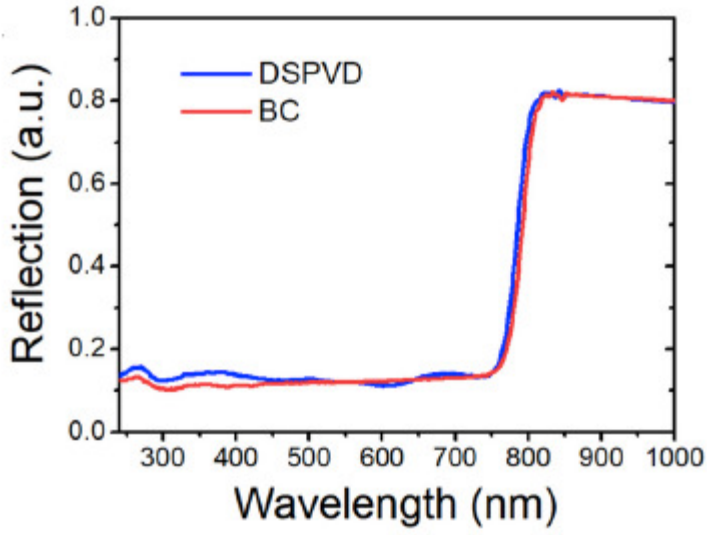

Fig.4. UV–Vis diffuses reflectance spectrum $MAPbI_3$ perovskite films.

2.3. Particle size distribution of PbI_2–DBEA (dibutylethanol amine)–MAI and PbI_2–DMSO (Dimethylsulfoxide)– MAI

Achieving high efficiency in perovskite solar cells requires the proper deposition of high-quality layers. The quick nucleation and crystallization of PbI_2, which causes large phase separation when a solvent evaporates during the film generation process, is one of the main problems with the quality of perovskite layers. Because of its distinct chemical structure, DBEA was chosen for this investigation as a multifunctional additive. DBEA, in contrast to other additives, consists of two hydrophobic chains and two hydrophilic groups (amine and hydroxyl). Therefore, it is anticipated that while its hydrophobic chains (butyl groups) may boost the solubility of well-coordinated Pb ions in a widely used solvent, its two hydrophilic groups may interact extensively with Pb ions (to create bigger clusters). We initially made PbI_2 solutions in a DMF solvent under ambient air conditions, both with and without DBEA, to confirm these hypotheses. As a point of comparison, we also made a PbI_2 solution using DMSO, which is a common solvent used in solvent engineering of perovskites [7].

Using a Zetasizer, the particle size distribution of the perovskite solution with DBEA was ascertained. The plot of dendritic architecture arising from tiny grains lining giant PbI_2 crystals is depicted in Fig. 5. Because of their greater solubility in DMF, these clusters are able to form a homogeneous film. These films are restructured by MAI soaking, which allows some DBEA to be exchanged for MAI molecules. Since DBEA is more soluble in CBZ than in MAI, CBZ wash aids in the completion of the DBEA exchange with MAI. Smaller perovskite clusters will interact with nearby crystals during this recrystallization process, forcing them to fuse together to produce a massive crystal grain.

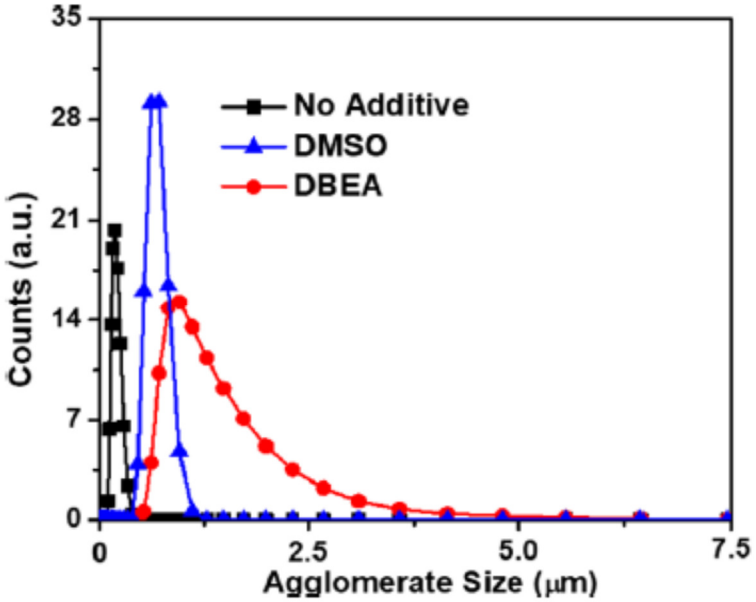

Fig. 5. PbI_2–DBEA–MAI and PbI_2–DMSO– MAI adduct clusters size distribution in precursor solutions in comparison to a pristine device without any additive.

The DBEA molecules will go to the surface or grain boundaries during this process, where they will interact with uncoordinated lead ions and defect locations to assist mitigate or passivate the defects. Furthermore, the nitrogen present in DBEA has the potential to substitute A-site vacancies on the perovskite surface, so contributing to the structural stability of the material. The PbI_2–DBEA–MAI adducts particle size distribution clusters in a solution with the optimal DBEA concentration. These graphs show that the DMSO-modified solution has a wider range with cluster sizes ranging from 300 nm to 1 μm, but the precursor solution with no additive has considerably smaller particles with a restricted size distribution (average particle size of 223 nm). The DBEA-incorporated solution showed a significant shift in particle size, with an average size of about 4 μm and some clusters showing sizes as high as 8 μm. These findings support our hypothesis that DBEA can interact with various Pb ions in solution to form different-sized clusters, and that these clusters determine the final product's shape.

Conclusion

The absorbance spectra of $CH_3NH_3PbI_3$ perovskite can be used to conceptualize the significant absorption in the visible region. Thin films' optical and structural characteristics suggest that there is still potential for solar photovoltaic applications. Films containing DBEA can be heated to produce homogenous, compact, extremely crystalline perovskite layers with grain sizes greater than 5 μm.

References

[1] Li H, Li F, Shen Z, et al. Photoferroelectric perovskite solar cells: Principles, advances and insights. Nano Today, 2021, 37: 101062

[2] Grätzel M. The light and shade of perovskite solar cells. Nature Mater., 2014, 13: 838-842.

[3] Jemli K. Synthése et Auto-assemblage de Molécules de Pérovskite Pour la Photonique et le Marquage, Université Paris-Saclay; Faculté des Sciences de Bizerte, Tunisie, 2016.

[4] Kour N, Mehra R. Recent Advances in Photovoltaic Technology based on Perovskite Solar Cell- A Review. J. Eng. Technol., 2017, 4(7): 1284-1296.

[5] Guo X, Mcleese C, Kolodziej C, et al. Identification and characterization of the intermediate phase in hybrid organic–inorganic $MAPbI_3$ perovskite†. Dalton Trans., 2016, 45: 3806-3813.

[6] Jeng J Y, Chen K C, Chiang T Y, et al. Nickel Oxide Electrode Interlayer in $CH_3NH_3PbI_3$ Perovskite/PCBM Planar-Heterojunction Hybrid Solar Cells. Adv. Mater., 2014, 26: 4107–4113.

[7] Yang W S, Noh J H, Jeon N J, et al. SOLAR CELLS. High-performance photovoltaic perovskite layers fabricated through intramolecular exchange. Science, 348: 1234–1237.