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Advances in Methylammonium Lead Halide Perovskites Synthesis, Structural, Optical and Photovoltaic Insights

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ABSTRACT

This study examines the structural, optical, and morphological characteristics of Methylammonium lead halide perovskites (MAPbX3) as potential solar cell candidates. Variable band gaps, extended carrier lifetimes, high absorption coefficients, and solution-processable synthesis techniques are among the numerous advantages of these perovskites. The Hot-Injection Method (HIM) is employed in the study to further investigate the unique properties of MAPbX3 perovskites, which is cost-effective and does not require vacuum. MAPbBr3 and MAPbCl3 crystallize in a cubic phase, whereas MAPbI3 crystallizes in a tetragonal phase. The halide versions exhibit morphological differences, with MAPbCl3 exhibiting cubic nanocrystals, MAPbI3 forming a combination of rods and spherical nanocrystals, and MAPbBr3 exhibiting particulate structures. TRPL experiments indicate carrier lifetimes between 1.72 and 7.65 ns, while UV-Vis spectroscopy indicates a blue shift in absorption band edges from MAPbI3 to MAPbCl3. MAPbI3, the most promising candidate for solar cell applications, produces a PCE of 13.66% at a thickness of 250nm, in contrast to MAPbBr3 and MAPbCl3, which produce 6.87% and 4.98% at a thickness of 500nm, respectively. This research establishes a thorough comprehension of the structural, optical, and morphological properties of MAPbX3 perovskites, thereby facilitating the advancement of perovskite solar cell technology and the creation of more cost-effective solar energy solutions.

Keywords: Methylammonium, Perovskites Solar Cells, MAPbX3, Photovoltaic, Hot-Injection Method.

INTRODUCTION

Methylammonium lead halide perovskites, namely $MAPbX_3$ (X = Cl, Br, I), have demonstrated potential as hybrid organic-inorganic perovskites in solar cell technology[1]. Perovskites provide appealing features such as extended carrier lifetimes, adjustable band gaps, strong absorption coefficients, and convenient synthesis processes that can be carried out using solutions. The optoelectronic characteristics of solar cells have led to a substantial increase in their power conversion efficiency (PCE), hence improving their competitiveness compared to traditional silicon-based cells. The perovskites $MAPbX_3$ have an ABX3 crystal structure, where X represents a halogen ion (Cl, Br, or I), B represents a smaller divalent cation (often lead), and A represents a larger monovalent cation (such as methylammonium, MA+). By altering the composition of the A, B, or X sites, the flexibility of this structure allows for the adjustment of several properties, including the band gap, absorption characteristics, and lattice parameters[3]. The Hot-Injection Method (HIM) synthesis of $MAPbX_3$ allows for the cost-effective and non-vacuum-based production of perovskites with distinct structural, morphological, and optical properties. This study aims to investigate the correlation between the structural characteristics of solar cells and their photovoltaic efficiency. It utilizes experimental research and device simulations to examine these attributes and their impact on the performance of solar cells. This study aims to provide a comprehensive understanding of the potential of $MAPbX_3$ perovskites for solar cell applications by utilizing photovoltaic simulations to evaluate their structural, optical, and morphological features[4]. The outcomes have the potential to guide future advancements in perovskite solar cell technology, hence promoting the development of more cost-effective and efficient solar energy alternatives[5].

EXPERIMENTAL METHODS

Methylammonium lead halide perovskites ($MAPbX_3$; X = Cl, Br, I) are synthesised using a number of important precursors to produce each variation. Lead salts, with 99.99% trace metals foundation, include lead(II) bromide ($PbBr_2$), lead(II) iodide (PbI_2), and lead(II) chloride ($PbCl_2$). The organic component is further made up of methylammonium halides, which include methylammonium iodide (MAI), methylammonium bromide (MABr), and methylammonium chloride (MACl), all of which are more than 99% pure. Important components of the solution chemistry, the solvents octadecene (ODE), oleyl-amine (OLA), and oleic acid (OA) stabilize the perovskites throughout production. Other compounds are also used especially in the manufacture of $MAPbI_3$, including tri-octyl phosphine (TOP). Consistency and purity in the produced perovskites are ensured by the usage of all chemicals, which are obtained from Sigma Aldrich and utilized directly[6].

The actual synthesis method is based on the controlled Hot-Injection Method (HIM). In a three-neck round-bottom flask (RBF), 1mM of MAI is dissolved in 3 mL of OA and well swirled. The solution is next rapidly injected with 0.5mM PbI_2 dissolved in TOP after being heated to 100°C in an argon atmosphere until clear. Following a ten-minute period at 195°C, the solution is chilled, centrifuged, and toluene-washed to produce $MAPbI_3$. With 1mM of MABr dissolved in a mixture of OA and ODE and $PbBr_2$ in the same mixture, the synthesis of $MAPbBr_3$ proceeds similarly[7]. The remainder of the process is 200°C, same as with $MAPbI_3$. The $MAPbCl_3$ synthesis is repeated at 180°C, with 1mM of MACl dissolved in the solution and $PbCl_2$ in an ODE and OLA mixture[8].

RESULTS AND DISCUSSION

The structural, optical, and morphological characteristics of the $MAPbX_3$ perovskites (X = Cl, Br, I) are evaluated through a thorough characterization process following their synthesis. Various techniques are employed to examine the properties of these perovskites[9]. X-ray diffraction (XRD) technique analyzes the crystalline structure, revealing information about each perovskite's phase, size, and lattice planes[10].

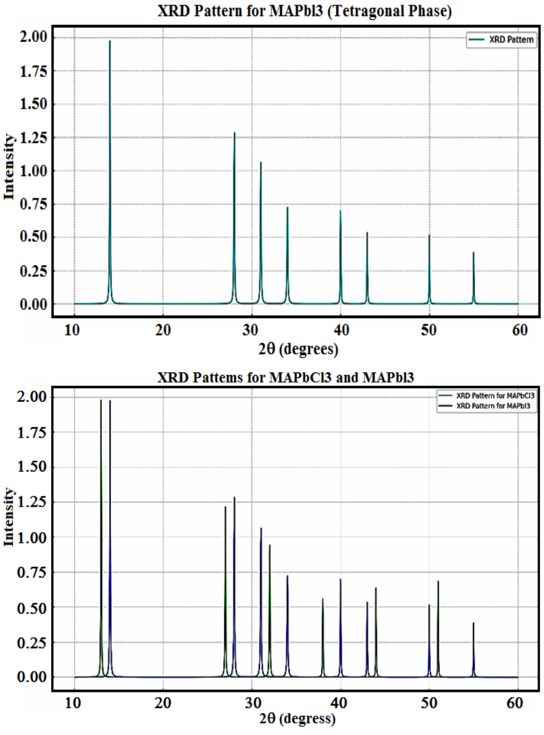

Fig. 1. XRD pattern of $MAPbBr_3$, $MAPbI_3$ and $MAPbCl_3$

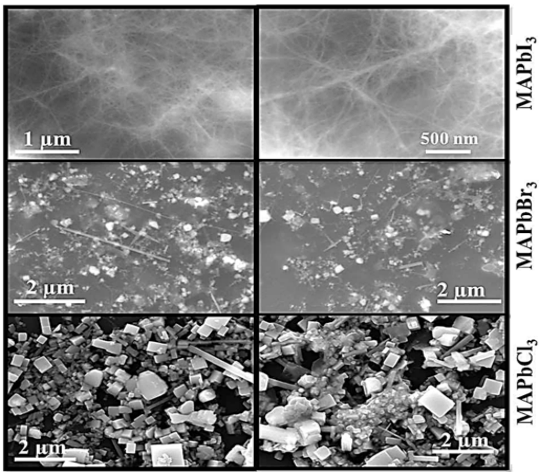

Fig. 2. SEM diagram of $MAPbI_3$, $MAPbBr_3$ and $MAPbCl_3$[7]

The diffraction patterns show that $MAPbBr_3$ and $MAPbCl_3$ crystallize in a cubic phase, while $MAPbI_3$ adopts a tetragonal phase[11]. The crystallite sizes range from 25.77 to 38.75nm, with lattice strains correlating with optical and photovoltaic properties. Field Emission Scanning Electron Microscopy (FE-SEM) imaging method provides insights into the surface morphology of each perovskite[12]. It captures particle shapes and distributions, revealing morphological variations between halide variants[13].

For instance, $MAPbI_3$ forms a mixture of rods and spherical nanocrystals, while $MAPbCl_3$ shows cubic nanocrystals, with particle sizes ranging from 31.1 to 44.5nm, in close agreement with the crystallite sizes calculated from XRD[14]. Transmission Electron Microscopy (TEM) technique provides high-resolution images of the perovskite particles, enabling a nanoscale analysis of their size and distribution. The particle size distribution can be computed from these images[15].

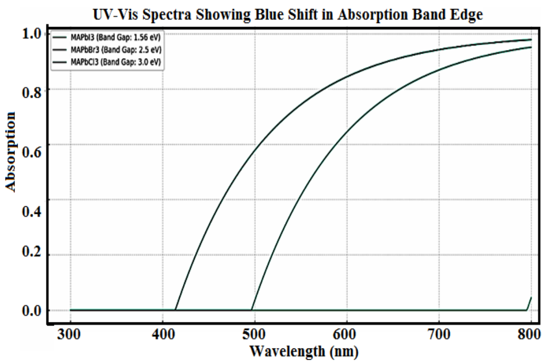

Fig. 3. Blue shifting in absorption band edge of $MAPbI_3$, $MAPbBr_3$ and $MAPbCl_3$

UV-Vis Spectroscopy This technique observes the absorption spectra of the perovskites, revealing band gaps and absorption coefficients[16]. The band gaps range from 1.56 to 3 eV, showing a blue shift in the absorption band edge from $MAPbI_3$ to $MAPbCl_3$. Photoluminescence (PL) investigations provide the emission spectra of the perovskites, showing broad peaks in the 400–800nm range, with blue shift emission from I through Br to Cl. Time-Resolved PL (TRPL) studies show carrier lifetimes of 1.72 ns ($MAPbI_3$), 1.87 ns ($MAPbBr_3$), and 7.65 ns ($MAPbCl_3$), indicating $MAPbCl_3$ has the longest charge separation. SCAPS-1D simulations show that $MAPbI_3$ yields a PCE of 13.66% at 250 nm thickness, while MAPbBr3 and $MAPbCl_3$ yield 6.87% and 4.98% at 500nm thickness, respectively[17]. The combination of band gap, carrier lifetimes, and photovoltaic efficiency positions $MAPbI_3$ as the most promising candidate for solar cells. Analysis and refinement of X-ray diffraction data (Analytical Technologies, India) using NetworkX Python library.

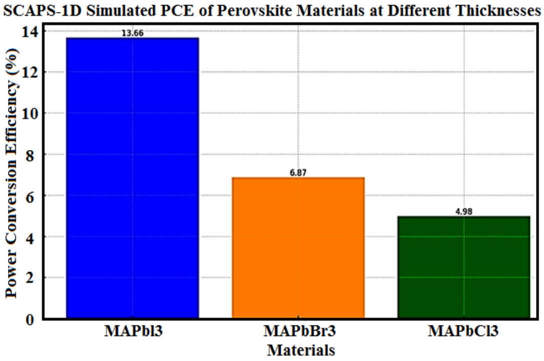

Fig. 4. SCAPS – 1D Simulated PCE of Perovskite Materials ($MAPbX_3$, X = Cl, I and Br) at different thicknesses

CONCLUSION

This study examines the potential application of methylaminium lead halide perovskites ($MAPbX_3$) in solar cell technology. The perovskites form distinct phases, with $MAPbI_3$ adopting a tetragonal morphology, while $MAPbBr_3$ and $MAPbCl_3$ have a cubic structure. The lattice strains are directly related to the optical and photovoltaic properties. The diameters of the crystallites vary between 25.77 and 38.75nm. Halide variants reveal distinct morphological variations; $MAPbI_3$ takes the shape of elongated rods and spherical nanocrystals, $MAPbCl_3$ showcases cubic nanocrystals, and $MAPbBr_3$ demonstrates granular structures. The UV-Vis spectroscopy revealed a blue shift in the absorption band boundaries when transitioning from $MAPbI_3$ to $MAPbCl_3$. The TRPL studies revealed carrier durations ranging from 1.72 to 7.65 ns, indicating that $MAPbCl_3$ has the most extended charge separation. $MAPbBr_3$ and $MAPbCl_3$ exhibited photovoltaic performance of 6.87% and 4.98%, respectively, when their thickness was 250nm. The study highlights the need of employing non-vacuum synthesis techniques, specifically the Hot-Injection Method (HIM), for cost-effective manufacturing of perovskites.

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Conflict of Interest

The authors conducted ethical and transparent research, demonstrating the importance of ethical practices in scientific research.

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