

# Review about Organic-Inorganic Perovskite Single Crystal : Synthesis Methods, Properties and Applications

Monik N. Maisuriya, Priyanka Desai

S.S Agrawal college of Commerce and Management, Navsari, Gujarat, India

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## ABSTRACT

Due to their easy synthesis and exceptional optoelectronic characteristics, such as their long carrier diffusion length, high carrier mobility, low trap density, and tuneable absorption edge ranging from ultraviolet (UV) to near-infrared (NIR), perovskite single crystals have attracted a lot of attention in recent years. These properties have the potential to be used in solar cells, photo-detectors (PDs), lasers, and other devices. In this review provides detailed information about the synthesis methods and applications of perovskite single crystals.

Keywords : Perovskite Single Crystal, Photo-Detectors, Solar Cell, Optoelectronic Properties

## I. INTRODUCTION

Calcium titanate ( $\text{CaTiO}_3$ ), which represents a specific form of crystal structure, was termed perovskite after the Russian mineralogist Count Lev Aleksvich Perovski. Organic-inorganic hybrid perovskite was initially described in 1978 and was discovered to have a similar structure to  $\text{CaTiO}_3$ . [1, 2] Metal halide perovskite crystal structure is generally denoted as  $\text{AMX}_3$ , where A is either organic or inorganic, M is the  $\text{Pb}^{2+}$  or  $\text{Sn}^{2+}$  cation and X is the halide anion (I, Br, and Cl). Metal hybrid perovskites have received a lot of attention due to their exceptional properties, which include broad absorption from visible to near-infrared as well as tuneable optical and electrical properties.

These findings show that perovskite single crystals are potentially useful building blocks. For photo-electric conversion applications. In this study, we focus on recent advances in the synthesis, characteristics, and applications of hybrid organic (in most cases) and all-inorganic (in some circumstances) perovskite single crystals. The exceptional performance of single crystals in applications like as PDs, solar cells, LEDs, and lasers is then demonstrated. Finally, the challenge and opportunity for perovskite single crystal applications are given.

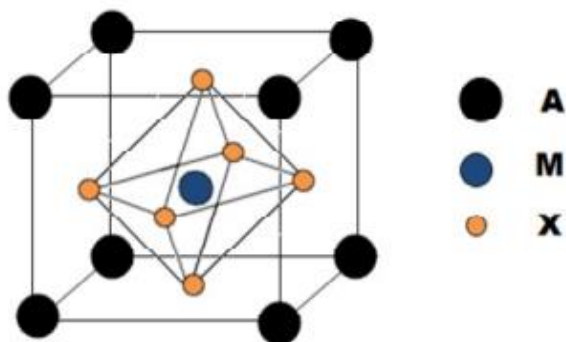


Figure.1 Crystal structure of perovskite ( $AMX_3$ ). [3]

## II. SYNTHESIS METHOD

In order to be used as a photovoltaic and photoelectric device, it is essential to synthesize high-quality perovskite single crystals under the right conditions and using the proper methods. Various methods have been employed in the past for synthesizing perovskite single crystals, but the challenge of producing large, high-quality crystals remains. The advancement of methods for synthesizing single crystals is a critical focus for researchers in the field. [4-7]

Traditional methods for synthesis perovskite single crystals include solution growth, solid-state reaction, and flux growth. Solution growth involves dissolving precursors in a solvent and then slowly cooling the solution to allow the crystals to form. Solid-state reaction involves reacting the precursors at high temperatures to form the perovskite crystals. Flux growth involves using a flux material to facilitate the growth of the crystals.

In recent years, several new synthesis methods have been developed to improve the quality and yield of perovskite single crystals. One promising method is the vapour-phase epitaxial, which involves depositing precursors onto a substrate and then heating them to form the crystals. Another method is the hydrothermal synthesis, which involves using high-pressure water to facilitate the formation of the crystals. These new methods offer greater control over the crystal growth process and can lead to the

synthesis of high-quality single crystals with tailored properties. [8-13].

Traditional methods take a so much time to grow a crystal compare to advance crystal growth method. Solution temperature lowering methods utilize a Webbers method. [14] In solution temperature lowering method dissolving precursors in a solvent and then slowly decrease a temperature. Bottom seed crystal growth and top seed crystal methods are types of solution temperature lowering method. Using this method synthesis a high quality hybrid perovskite crystal. (Shown in figure.2)

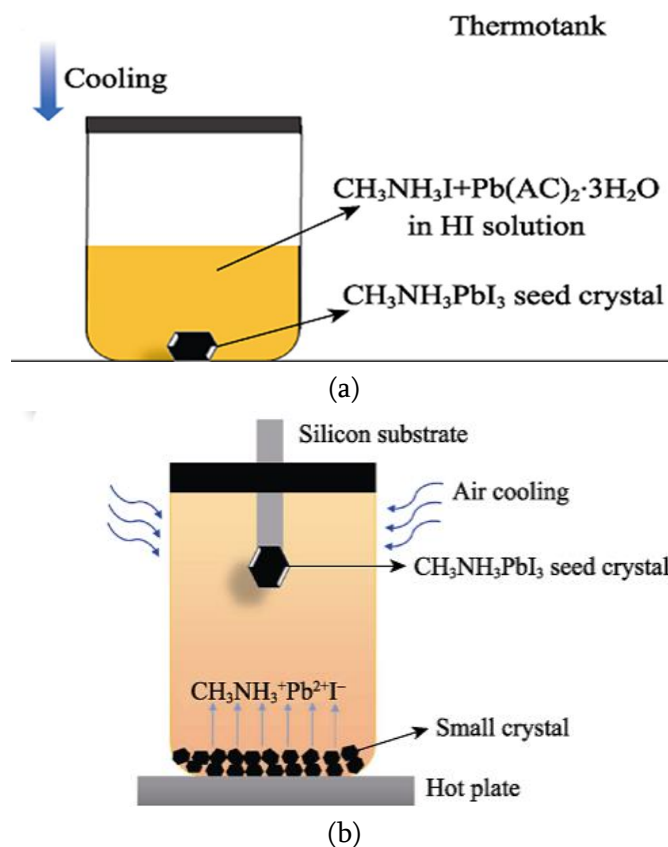


Figure. 2 Schematic diagram of solution temperature-lowering crystallization (STL) (a) Crystallization process of BSSG and images of as-prepared  $CH_3NH_3PbI_3$  single crystal (b) Crystallization process of TSSG and image of as-prepared  $CH_3NH_3PbI_3$  single crystal.[15]

Advance method like a anti-solvent vapour assisted crystal growth, thickness controllable crystal growth

and inverse temperature crystallization method is take less time and fast crystal growth method. [16]

In anti solvent method is base on solubility of the precursor solution in different solvent to synthesis of high quality perovskite crystal in reproducible and independent to temperature manner. In recent years Bakers group a synthesis a defect free high quality perovskite crystal. (Shown figure.3)

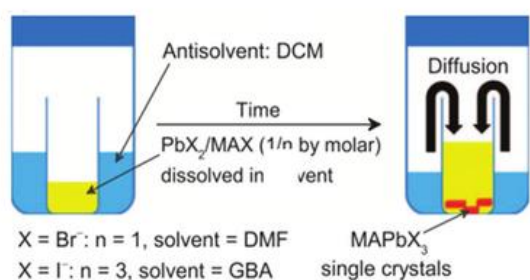


Figure.3 schematic diagram of the AVC method. [17]

In Inverse temperature crystallization method the initial solution placed in a container and subjected to heat as part of inverse temperature crystallization (ITC) technique. As the solvent evaporates, the upper part of the solution becomes saturated during the crystal growth stage, while the lower part remains unsaturated. The ITC method, various types of perovskite single crystals such as MAPbI<sub>3</sub>, MaPbBr<sub>3</sub> and FAPbI<sub>3</sub> are synthesis. [18]

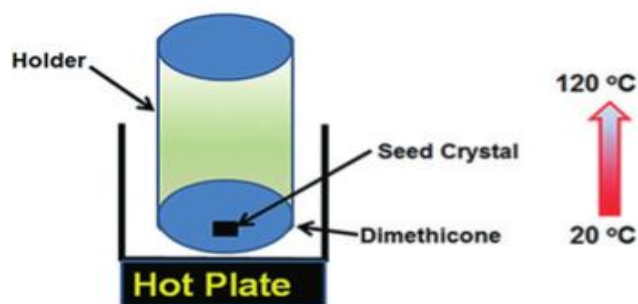


Figure.4 Schematic diagram of Crystallization process of ITC and images of as-prepared CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> single crystal.[19]

Another recent advance method is Thickness controllable method. Achieving precise thickness control has proven to be a hurdle in the advancement of perovskite synthesis techniques. The thickness of individual crystals plays a crucial role in determining the functionality of the device they are incorporated into. By using this method at room temperature control a development and thickness of perovskite crystal. By using this method it possible to synthesis of 2D perovskite crystal.[20]

### III.PROPERTIES

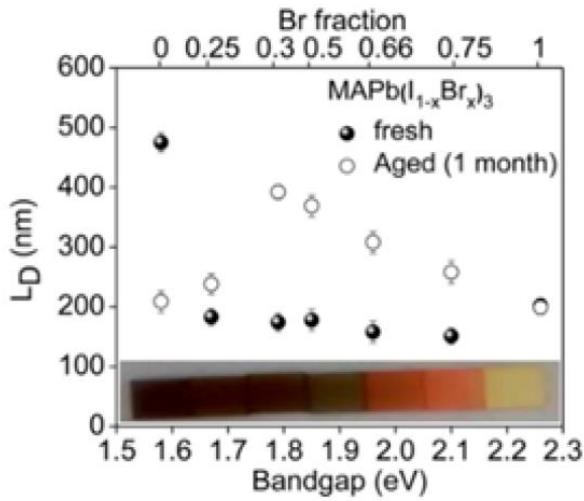
Perovskite crystals belong to a category of materials with intriguing optical and electrical characteristics that make them appealing for a wide range of applications.[21-23]

#### 3.1 OPTICAL PROPERTIES

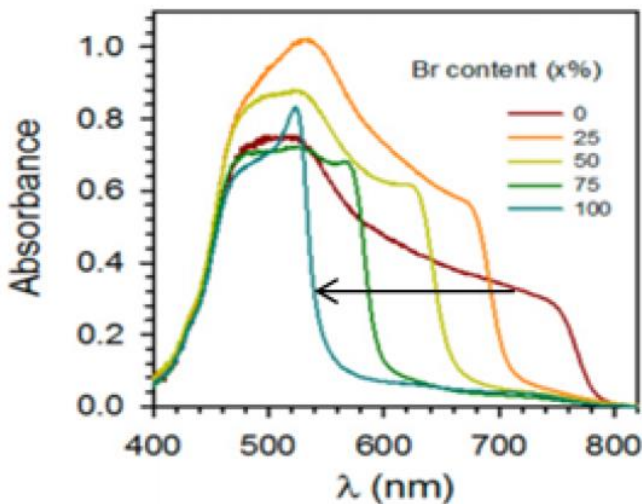
In terms of optical properties, perovskite crystals possess a high absorption coefficient, making them efficient for use in solar cells. This feature allows for the use of thin films in solar cell applications, while also exhibiting strong photoluminescence that is ideal for light-emitting devices. The tuneable band-gap of perovskite crystals enables the optimization of their optical properties for specific applications, and their high quantum yield results in efficient light emission. This makes them promising candidates for use in lasers and light-emitting diodes. [24]

Hybrid perovskite semiconductors exhibit direct-band-gap characteristics, resulting in significant absorption coefficients ranging from 10<sup>4</sup> to 10<sup>5</sup> cm<sup>-1</sup>. [25, 26] The point at which absorption begins provides valuable insight into the optical band-gap of a material. Additionally, the sharpness of this absorption onset and the existence of a tail below the absorption edge can indicate the quality of the material. [27, 28] This quality is often linked to the presence of imperfections and defects within the material. [29, 30] Spectrum absorption can also reveal

information about the nature of photo-generation. (Show In figure 5).



(a)



(b)

Figure.5 (a) A plot of diffusion length (L nm) against bandgap energies aged and non aged MAPb(I<sub>1-x</sub>Br<sub>x</sub>)<sub>3</sub> Perovskite crystal.(b) Absorption spectra of mixed halide perovskite crystal. [31]

### 3.2 ELECTRICAL PROPERTIES

When it comes to electrical properties, perovskite crystals have high carrier mobilities, enabling efficient charge transport which is essential for the performance of perovskite based photovoltaic devices.

These crystals also demonstrate low trap densities, leading to high carrier lifetimes and contributing to the high efficiency of perovskite solar cells. Additionally, perovskite crystals exhibit excellent charge separation and collection properties, resulting in high photovoltaic performance in solar cell applications. [32-37] typically, the SCLC approach was used to examine single-crystal conductivity, carrier mobility, and carrier diffusion length. [38].

The dark current-voltage (I-V) curve is really measured using this technique by manufacturing the metal/single-crystal wafer/metal structure. Three regions of the curve can be identified: the Ohmic zone, the trap-filled region, and the Child's region. The formula  $\sigma = I/(VL)$  can be used to determine the conductivity from the Ohmic region's curve. The following equation can be used to compute the trap density:

$$n_t = \frac{2\epsilon\epsilon_0 V_{TFL}}{eL^2} \quad (1)$$

Where  $e$  is the elementary charge,  $L$  is the thickness of a single crystal,  $\epsilon_0$  is the vacuum permittivity and,  $\epsilon$  is the relative permittivity. The  $V_{TFL}$  is the point of the trap-filled zone and the Ohmic-region. By measuring capacitance and frequency, it is possible to determine the relative dielectric constant. As dopants, traps in single crystals affect the conductivity and carrier diffusion length of the electronic characteristics. The traps for thin films are dispersed around the grain boundaries, in the bulk, and on the surface. The traps are largely spread on the surface and bulk of single crystals, albeit there are hardly any grain boundaries in these structures. In contrast to thin films ( $10^{14} \text{Cm}^{-3}$  to  $10^{13} \text{Cm}^{-3}$ ), there are thus fewer trap densities ( $10^{10} \text{Cm}^{-3}$ ). Mott-Gurney's law, which was established by the following equation [39], can be used to compute the carrier mobility ( $\mu$ ) in the Child area ( $n=2$ ):

$$\mu = \frac{8L^3 J_D}{9\epsilon\epsilon_0 V_b^2} \quad (2)$$

Where  $V_b$  stands for the voltage that is being used and  $J_D$  is the current density. The transmission rate of electrons and holes per voltage, which is affected by traps, is represented by the carrier mobility. Another crucial parameter is the diffusion length ( $L_D$ ), which is calculated using the carrier mobility  $\mu$  and carrier lifetime  $\tau$ . The formula is as follows:

$$L_D = \sqrt{\frac{k_B T \mu \tau}{e}} \quad (3)$$

Where  $T$  is the temperature and  $k_B$  is the Boltzmann constant. According to the prior findings, the carrier diffusion length for crystals is between 3  $\mu\text{m}$  and 3 mm. The contact resistance and strong electric field, however, demonstrate that the estimated diffusion length exists with a small variation.

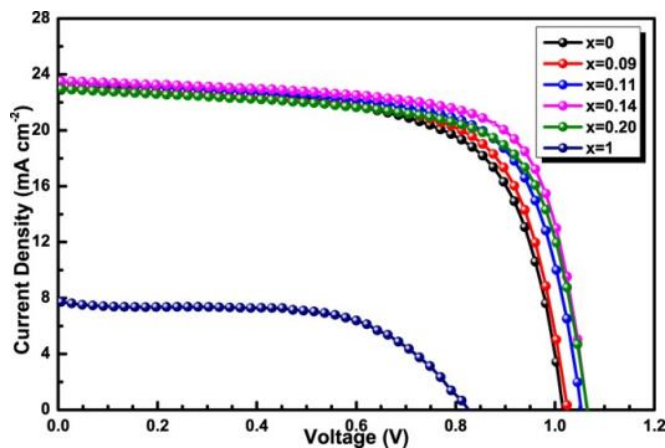


Figure.6 J-V characteristics of the MAPbI<sub>3-x</sub>Br<sub>x</sub> cells [40]

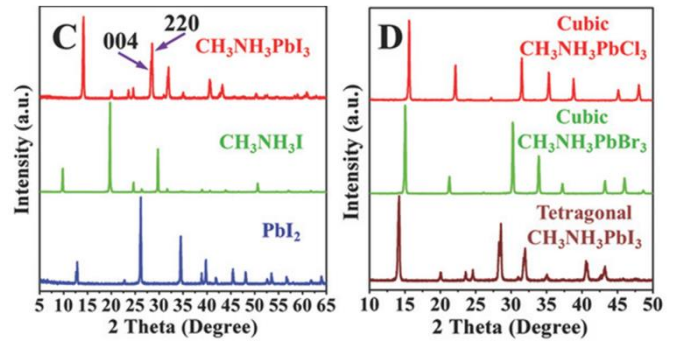
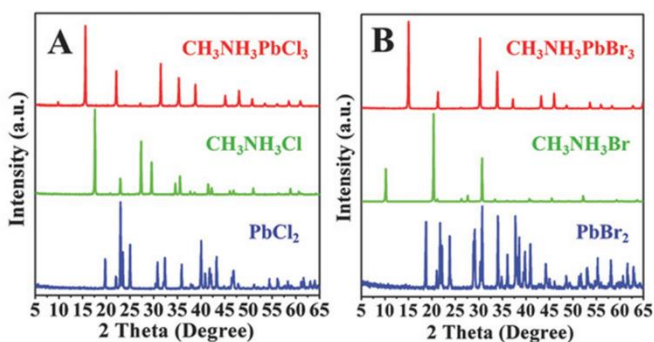


Figure. 7 X-ray diffraction patterns of the ground powder from large CH<sub>3</sub>NH<sub>3</sub>PbX<sub>3</sub> single crystals, A) X = Cl, B) X = Br, C) X = I, D) the XRD comparison of three perovskites. [41]

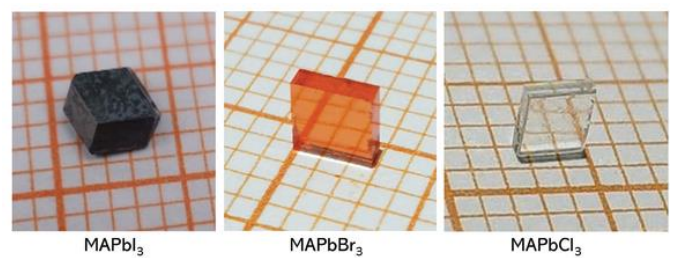


Figure.8 Photographic images of single crystals MAPbX<sub>3</sub> (X = I, Br, Cl) single crystals.[41]

#### IV.APPLICATION

Perovskite crystal is a type of material known for its distinct crystal structure and has attracted significant attention in a wide range of industries. Its exceptional properties make it suitable for various applications. In the realm of solar energy, Perovskite crystals have displayed remarkable efficiency in converting sunlight into electricity.[42] This breakthrough could potentially transform the renewable energy sector. Furthermore, Perovskite crystals have been successfully integrated into LED technology, producing bright and energy-efficient light sources.[43-46] This innovation may lead to more sustainable lighting solutions in the future. In sensor applications, [47-51] Perovskite crystals have demonstrated high sensitivity to different stimuli, promising improved accuracy in sensor devices. Exploration into the use of Perovskite crystals in quantum computing has shown promise. [52-56] their

unique characteristics could enhance the performance of quantum computers, paving the way for advancements in computing technology.

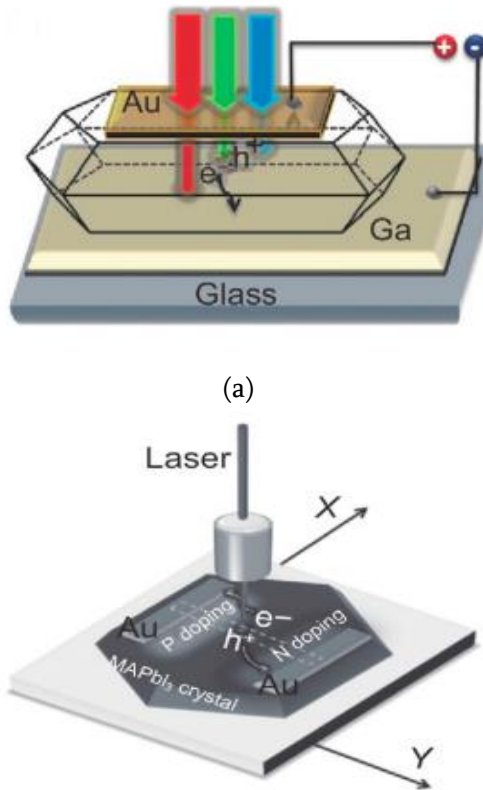


Figure.9. Solar cells based on perovskite single crystals: (a) vertical structure device architecture of PSC based on the MAPbI<sub>3</sub> single crystal ;(b) schematics of lateral structure solar cells [57]

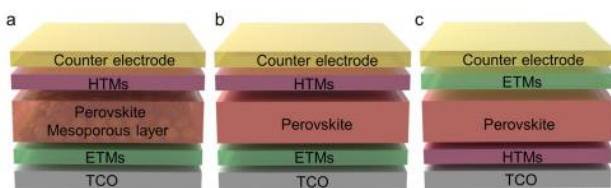


Figure.10 Device structures of PSCs. (a) Mesoporous structure. (b) Regular n-i-p structure. (c) Planar p-i-n (inverted) structure[58]

## V. CONCLUSION

In review, we have detailed the development and formation of perovskite single crystals, as well as their unique properties and practical applications. The ability of precursor materials to dissolve in different solvents and the methods for producing top-notch

perovskite single crystals have been summarized as being influenced by temperature variations.

We present a comprehensive overview of the fundamental optical, transport, and photo physical properties that influence the functionality of perovskite based optoelectronic devices. Key factors such as band-gap, mobility, diffusion length, charge-carrier lifetime, and defect-trap density play a crucial role in determining device performance.

In the ABX<sub>3</sub> structure, each site has the potential for substitution or doping with two or three different components. For instance, replacing Pb with metals like Sn or Bi at the B site can result in the creation of non-toxic single crystals. Photoluminescence (PL) characteristics in single crystals are distinct from those in thin films, primarily due to the higher purity of single crystals. Understanding these differences can help in reducing traps and optimizing device performance in specific application environments.

The use of high-quality perovskite single crystals can significantly enhance the efficiency of advanced devices such as LEDs, photodiodes, and solar cells. Additionally, their incorporation simplifies device designs and streamlines production processes using various fabrication techniques. Exploring and optimizing carrier multiplication properties in perovskite single crystals can lead to the generation of a higher density of efficient carriers, thereby improving overall device performance. In conclusion, the versatility and value of Perovskite crystals across multiple industries are undeniable. Continued research and development in this field will undoubtedly unlock even more potential in the future.

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