Structural properties of perovskite thin film

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Abstract

Methyl-ammonium lead tri iodide ($CH_3NH_3PbI_3$) have been attracted attention in the domain of solar energy because of their great absorption coefficient and little temperature fabrication. Perovskite thin film have been prepared by solution processing. Thin film after dropped in the laboratory ambient states by drop casting, it made by two step procedure PbI_2 and CH_3NH_3I at the glass substrates. The analysis deals the structural properties, x-ray diffraction, and scanning electron microscope of these films with tetragonal structure. Space group I4/mcm (Z=4), a=8.800 Å,c=12.685 Å ،crystallite size was 340 nm, dislocation density 8.19 $\times 10^{-4}$ lines/m^2 and micro strain 9.93 $\times 10^{--8}$ $lines^{-2}/m^4$.

Key words: Structural properties, perovskite, drop casting, two step method.

الخلاصة

مثيل امونيوم ثلاثي ايوديد الرصاص $CH_3NH_3PbI_3$ حاز على اهتمام واسع في مجال الطاقة الشمسية وذلك لامتلاكه معامل امتصاص عالي وتصنيعه في درجات حرارة واطئة، ان الأغشية الرقيقة لمادة البيروفسكايت تم تحضيرها بطريقة الاذابة على مرحلتين تحت الظروف المختبرية من خلال مادتي PbI_2 و CH_3NH_3I على القواعد الزجاجية.الفحوصات التركيبية كانت من خلال فحص XRD

والطوبوغرافية من خلال فحص SEM لهذه الاغشية ذات التركيب الرباعي ومجموعة فضاء I4/mcm (Z=4) بابعاد a=8.800 Å, c=12.685 Å ،فكان الحجم الحبيبي 340 nm ، كثافة الانخلاعات 8.19×10^{-4} lines/m² بينما كانت الانفعالات المايكروية 9.93×10^{-8} lines^{-2}/ m^4 lines^{-2}/ m^4 . كما أظهرت صورة SEM الشكل المكعب للنموذج المحضر.

1. Introduction

Methyl-ammonium Lead (or Tin) Tri-halide ($CH_3NH_3PbX_3$, CH_3 NH_3 Sn X_3; X = Cl, Br, I) organic-inorganic hybrid perovskite thin films are excellent high-ranking semiconductors saw till date[1].These are deliberated as appropriate materials for designing great performance photovoltaic devices because these are having extremely large potential to convert the Sun's photon energy into electricity[2],an final source for future energy from renewables. Efforts to inspect this specific light conversion feature by diverse research groups have thrived in leaps and bounds, reaching to a National Renewable Energy Laboratory specialized Power Conversion Efficiency (PCE) of 22.1% [3].methyl-ammonium lead tri-iodide ($CH_3NH_3PbI_3$, also known as $MAPbI_3$) has developed from an firstly reported value of 3.8% to a National Renewable Energy Laboratory specialized value of 22.1% within a few years. Such a development of the PCE has really taken periods for other photovoltaic solar cells to achieve [4]. However, the amazing and highly superior design principles and synthetic ways exposed during the study of the $CH_3NH_3PbX_3$ and their halogen derivatives are indicated to contribution the creation of the next generation tri halide based perovskite solar cell materials[3].Graetzel and co-workers have showed the use of the two-step deposition technique as a influential technique for attaining highly efficient perovskite solar cells [5]. The two-step deposition lets better control over the perovskite crystallization by separating the perovskite deposition into the two precursors ((two-step)). Density Short Current (J_{sc}) is eventually controlled by the optical absorption in the solar cell absorber layer. So, determination and clarification of $CH_3NH_3PbI_3$ optical properties are of critical importance for the further growth of $CH_3NH_3PbI_3$ solar cells. It is known well that $CH_3NH_3PbI_3$ is a direct transition semiconductor[6].An addition for perovskite SCs, organic-inorganic perovskite are also talented materials for light-emitting diodes [7], lasers[8] and thin film electronic devices[9].

The Aim of this research is synthesis perovskite material $CH_3NH_3PbI_3$ Then study properties of perovskite thin film

2. The Crystal Structure Form and Formation

The parameters and transitions of phases of bulk $MAPbI_3$ were concerned in references [10,11]. Here, we emphasis on the tetragonal and cubic phases [12]. In fact, there are no critical alterations between the two phases, but a small rotation of PbI_6 octa-hedra along the c-axis. The atomic structures of $MAPbI_3$ of the two phases are shown in Figure 1 (A,B). Thus, the tetragonal phase can be preserved as a pseudo cubic phase [13]. Below 54 ^{0}C, the cubic phase of $MAPbI_3$ can be transformed into the tetragonal phase [10] , and the opposite transition occurs by annealing at 100 ^{0}C for 15 min [14].

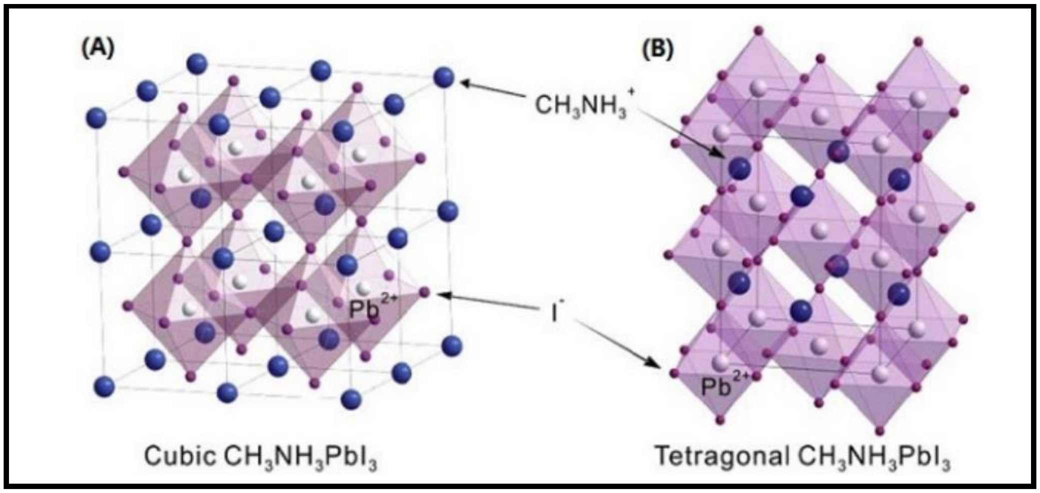

Fig.1 :Crystal Structure of $CH_3NH_3PbI_3$

3. Structural Characterization of the films

Perovskites with ABX_3 – structure show a huge option on element replacements on A^-,B^- and X-site which leads to a wide variety of physical properties. In latest years the care become focused on hybrid perovskites as a future photovoltaic material. Our field of attention places in lead methyl-ammonium tri-iodide in which A is the organic unit $[CH_3NH_3]^+$, $B=Pb^{2+}$ and $X=I^{3-}$. The diverse perovskite crystal structures can be ordered by their octahedral coordinated B cation. The aristo type-structure (P m-3m) is symmetry lowered due to tilting, distortion of $[BX_6]$ - octahedra or displacement of B^-cation from center of octahedron. [16]. Among all the present analytical techniques applied to examine the line broadening of X-ray diffraction, the Scherrer method[17] is a greatest easy formulation and therefore still used to valuation the "apparent" domain sizes of physical broaden peak profile. This method describes the crystallite size in terms of a mean effective size of the coherently scattering region normal to the reflecting planes[18]. The Scherrer relation between crystallite size and integral breadth is given by:

$$D = \frac{K\lambda}{\beta\ COS\ \Theta} \dots\dots\dots\dots\dots\dots\dots \quad (1)$$

where, D is the effective crystallite size normal to the reflecting plane, K is a shape factor (K = 0.9), λ is the wavelength of Cu Kα radiation, β is the integral width of a particular peak and θ is the diffraction angle. From equation (1) it is clear that size broadening is liberated of order of a reflection. The dislocation density (δ), defined as the length of dislocation lines per unit volume of the crystal, is expected from the formula [19] .

$$\sigma = \frac{1}{D^2} \dots\dots\dots\dots\dots (2)$$

The strain made peak broadening resulting from lattice distortion (microstrain) can be stated by Wilson formula [20]:

$$\eta = \frac{\beta\ COS\ \Theta}{4} \dots\dots\dots\dots\dots\dots\dots\dots. (3).$$

4. Materials and Methodolgy

Synthesis of organic perovskite materials (OPM) reported in reference [15]. Methylamine Iodide (CH_3NH_3I) is prepared by reacting Methylamine, 33% of weight in ethanol (BDH-LTD), with Hydro-Iodic acid (HI) 57% of weight in water (BDH-LTD) under ice bath stirring for 2 h. Typical quantities employed are 24 ml of Methylamine, 10 ml of HI, and 100 mL of ethanol then stirrer at 100 °C, a transparence solution is formed.

5. Results and Discussions

5.1 XRD

Figure (2) depicts the XRD pattern of $CH_3NH_3PbI_3$ layer achieved by deposited perovskite precursor solution using drop casting and annealing at 150oC. All reflections is indicated to the tetragonal $CH_3NH_3PbI_3$. Reflections positions of (200), (211), (202), (004), (220), (114), (310) (312), (321) (400) (314) (420) , (404) , (424) and (440), the result in agood agreement with [21] corresponding with tetragonal structure Space group I4/mcm (Z=4), a=8.800 Å,c=12.685 Å are indicated by ref [6, 21] for comparative .

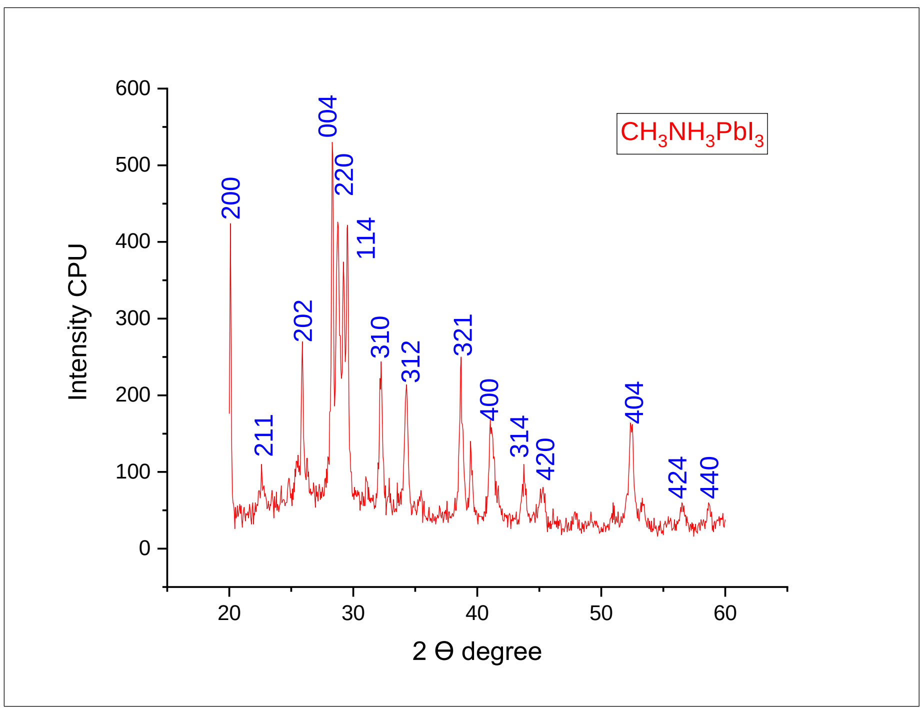

Fig.2 XRD of $CH_3NH_3PbI_3$ film.

The other parameters are shown in table 1.

Table 1: Some structural parameters of $CH_3NH_3PbI_3$ film.

D **crystallite size** nm	***σ*** **dislocation density** lines/m^2	***H*** **micro strain** $lines^{-2}/ m^4$
34،	8.19×10^{-4}	10×10^{-8}

5.2 SEM

Figure (3) is shows the top SEM image of $CH_3NH_3PbI_3$ film ,is displayed SEM image of $CH_3NH_3PbI_3$ layer on glass substrate that have crystal growths with more cubic shape of the film up to 1 μ m. scale bars of the image is 10 µm, scanning with high voltage 5kV and magnification 5 kx. Samples are prepared by deposited perovskite precursor solution using drop casting at 100^0C preheated sheet glass substrate ,good agreement with [23],[24].

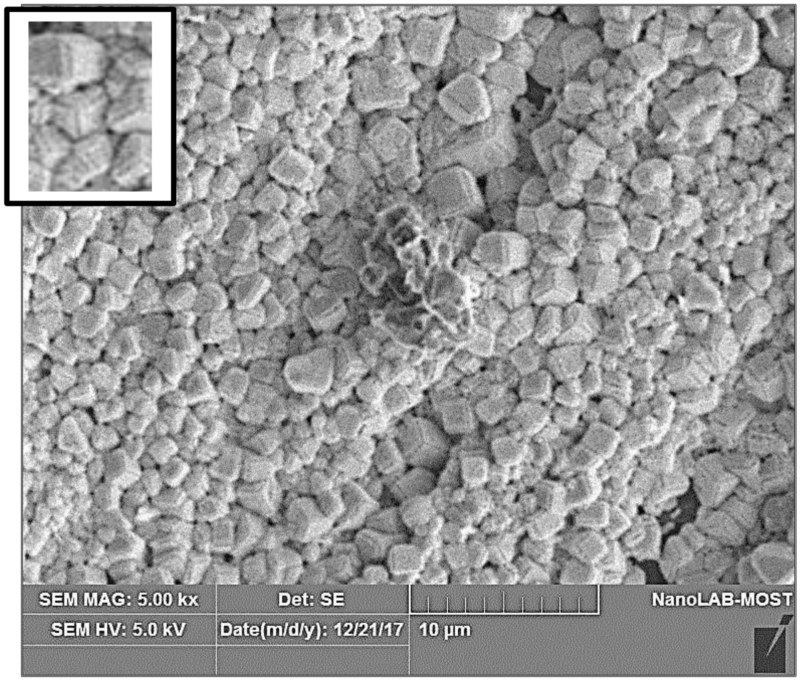

Fig.3 SEM of $CH_3NH_3PbI_3$ thin film.

Conclusions

In this work, it has been studied the structural properties of $CH_3NH_3PbI_3$ thin films after deposited in the laboratory ambient situations by drop casting, it prepared by two step process, thin films have been made by solution processing have tetragonal structures ,Space group I4/mcm (Z=4), a=8.800 Å,c=12.685 Å with more cubic shape. SEM have been shown cubic shape of the sample.

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